

## Supporting Information

# Reactivity of a Series of Isostructural Cobalt Pincer Complexes with CO<sub>2</sub>, CO, and H<sup>+</sup>

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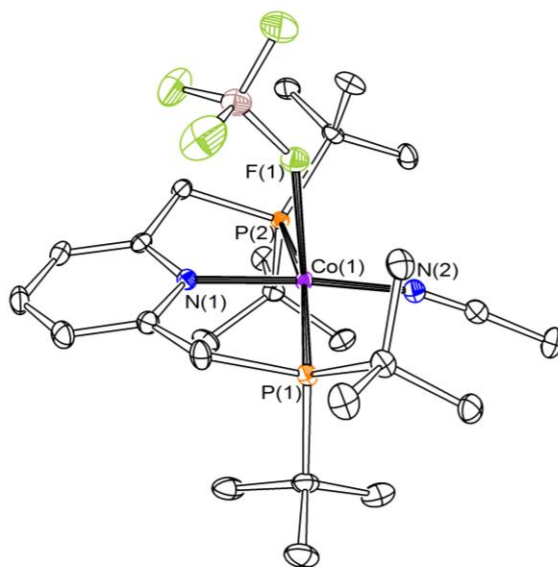
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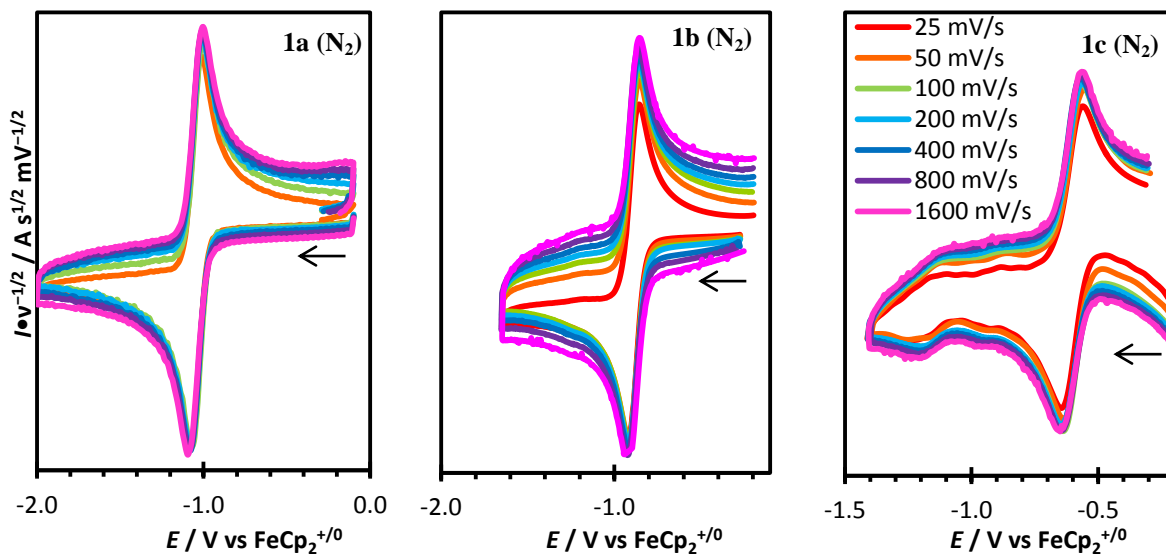
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**Table S1. X-ray Diffraction Data Collection and Refinement Parameters**

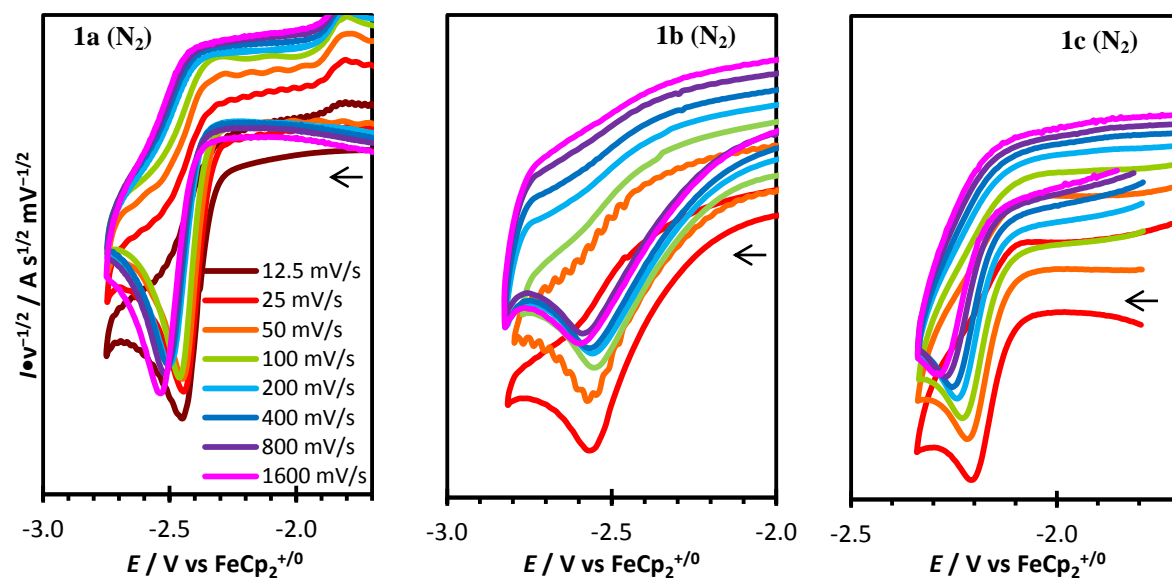
|  | $[(P^C N^C P)Co(NCCH_3)(BF_4)][BF_4]$ ( <b>1a</b> ) | $[(P^C N^C P)Co(NCC H_3)_2][BPh_4]_2$ ( <b>1a'</b> ) | $[(P^N N^N P)Co(CH_3CN)_2](BF_4)_2$ ( <b>1b</b> ) | $[(P^C N^C P)Co(NCCH_3)][BF_4]$ ( <b>2a</b> ) | $[(P^N N^N P)Co(NCCH_3)][BF_4]$ ( <b>2b</b> ) |
|--|---|--|---|---|---|
| Empirical formula  | $C_{25}H_{46}B_2CoF_8N_2P_2$                        | $C_{77}H_{92}B_2CoN_4P_2$                            | $C_{27}H_{50}B_2CoF_8N_6P_2$                      | $C_{26}H_{46}BCoF_4NP_2$                      | $C_{23}H_{44}BCoF_4N_4P_2$                    |
| Formula weight   | 669.13  | 1216.04  | 753.22  | 580.32  | 584.30  |
| Crystal system   | Monoclinic  | Triclinic  | Monoclinic  | Triclinic                                     | Orthorhombic                                  |
| Space group  | $C2/c$  | $P\bar{1}$   | $P2_1/n$  | $P\bar{1}$                                    | $Pnma$  |
| $a / \text{\AA}$   | 31.694(6)   | 13.2293(8)   | 12.0102(4)  | 11.9513(18)                                   | 16.299(2)                                     |
| $b / \text{\AA}$   | 9.9983(19)  | 13.8571(8)   | 25.2799(9)  | 15.225(2)                                     | 21.997(3)                                     |
| $c / \text{\AA}$   | 19.793(4)   | 21.5246(12)  | 13.1060(5)  | 32.953(5)                                     | 32.508(4)                                     |
| $\alpha / \text{deg}$  | 90  | 82.306(3)  | 90  | 90.5946(19)                                   | 90  |
| $\beta / \text{deg}$   | 94.329(4)   | 73.106(3)  | 114.6170(10)                                      | 93.9705(17)                                   | 90  |
| $\gamma / \text{deg}$  | 90  | 63.583(3)  | 90  | 90.0638(17)                                   | 90  |
| $V / \text{\AA}^3$   | 6254(2)   | 3381.3(3)  | 3617.5(2)   | 5981.3(16)                                    | 11655(3)                                      |
| $Z$  | 8   | 2  | 4   | 8   | 16  |
| Refl. Collected  | 25223   | 69216  | 39505   | 63394   | 131238  |
| Indep. Refl.   | 6402  | 13884  | 7409  | 24252   | 13202   |
| R1 ( $I > 2\sigma$ ) <sup>a</sup>  | 0.0263  | 0.0418   | 0.0287  | 0.1120  | 0.0508  |
| wR2 (all data) <sup>b</sup>  | 0.0667  | 0.0987   | 0.0378  | 0.3216  | 0.1452  |
| <sup>a</sup> R1 = $\sum   F_o  -  F_c   / \sum  F_o $ . <sup>b</sup> wR2 = $\{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$ . |   |  |   |   |   |



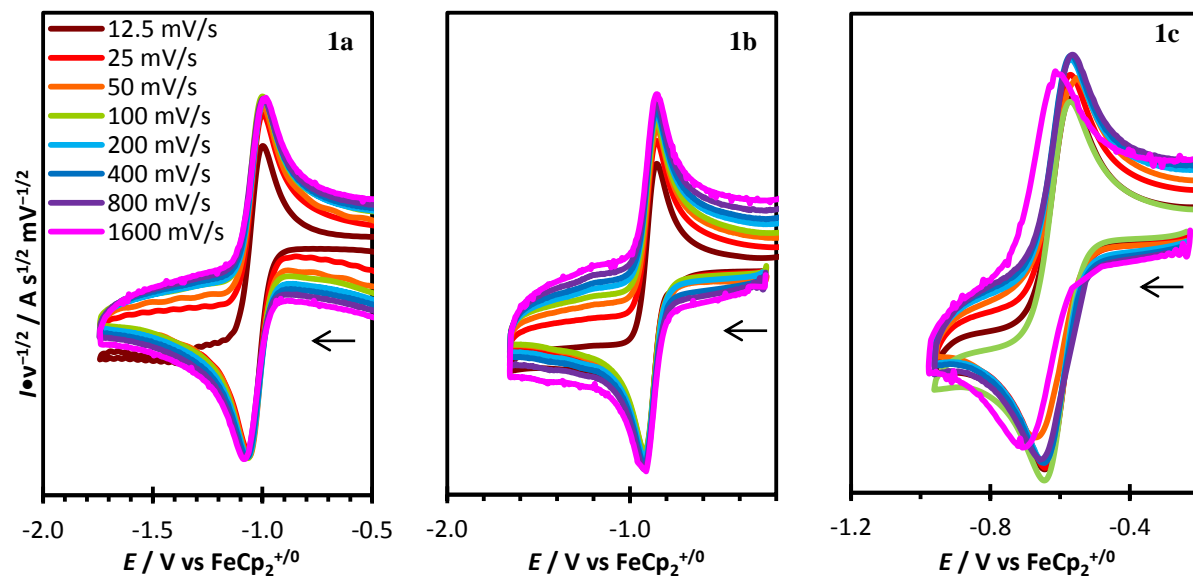
**Figure S1.** ORTEP diagram of  $[(P^C N^C P)Co(NCCH_3)(BF_4)][BF_4]$  (**1a**). Ellipsoids are shown at 50% probability. Hydrogen atoms and outer-sphere  $BF_4$  anion have been omitted for clarity.



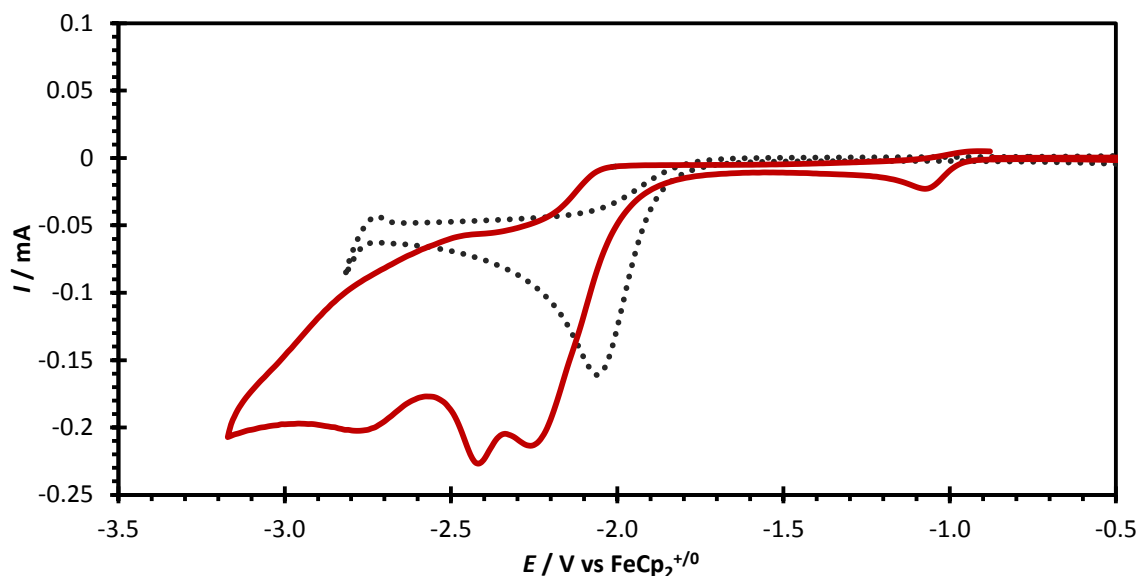
**Figure S2.** Cyclic voltammograms of the first reductions of  $[(P^E N^E P)Co(NCCH_3)_2][BF_4]_2$  (E = C, **1a**, left; N, **1b**, middle; O, **1c**, right) under  $N_2$  at various scan rates. Current is normalized by square-root of scan rate. 1.0 mM analyte in  $CH_3CN$  with 0.20 M  $Bu_4NBF_4$ . Arrows indicate the scan direction and the position of the bulk material.



**Figure S3.** Cyclic voltammograms of the second reductions of  $[(P^E N^E P)Co(NCCH_3)_2][BF_4]_2$  ( $E = C$ , **1a**, left;  $N$ , **1b**, middle;  $O$ , **1c**, right) under  $N_2$  at various scan rates. Current is normalized by square-root of scan rate. 1.0 mM analyte in  $CH_3CN$  with 0.20 M  $Bu_4NBF_4$ . Arrows indicate the scan direction.

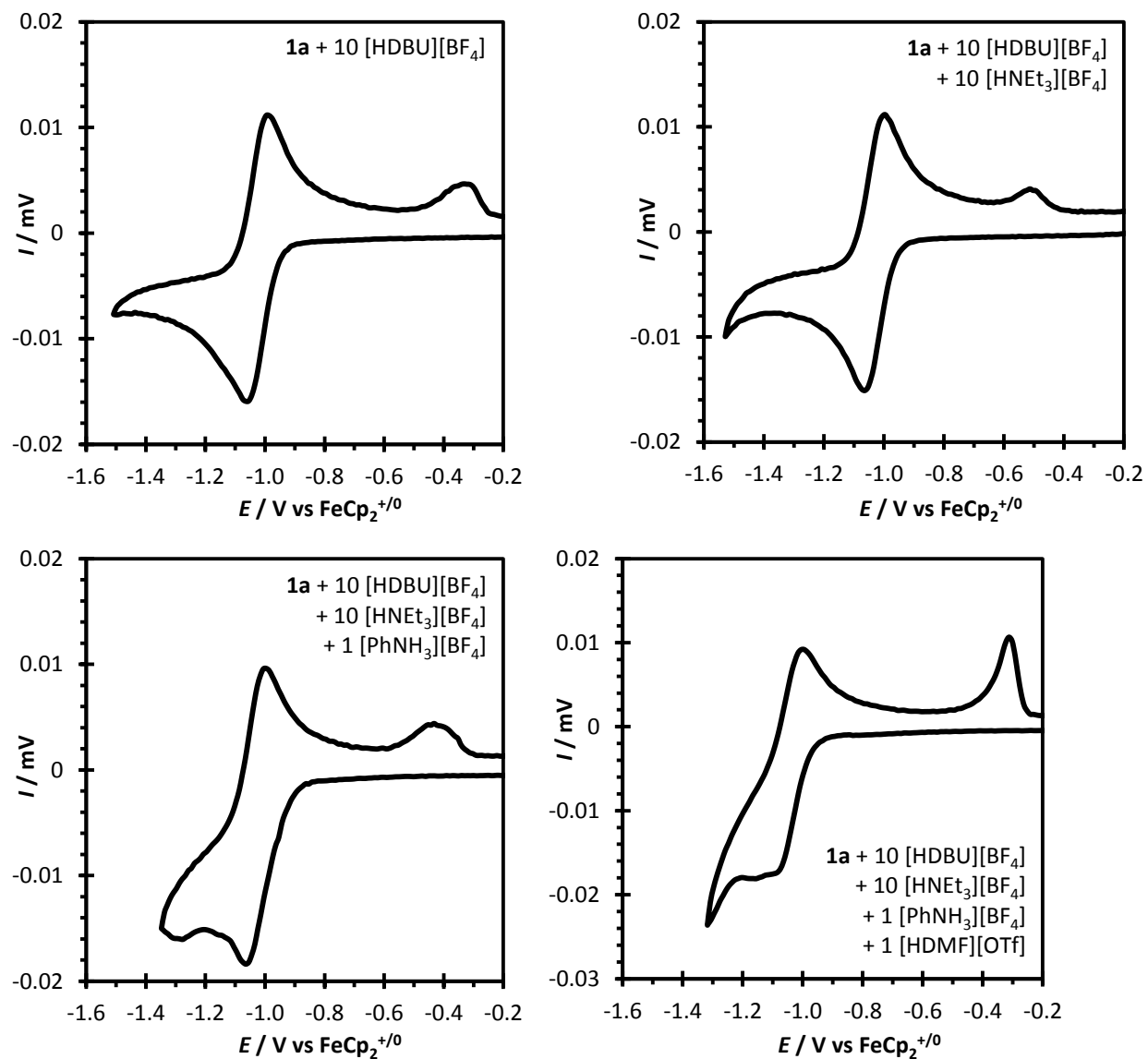


**Figure S4.** Cyclic voltammograms of the first reductions of  $[(P^E N^E P)Co(NCCH_3)_2][BF_4]_2$  ( $E = C$ , **1a**, left;  $N$ , **1b**, middle;  $O$ , **1c**, right) under  $CO_2$  at various scan rates. Current is normalized by square-root of scan rate. 1.0 mM analyte in  $CH_3CN$  with 0.20 M  $Bu_4NBF_4$ . Arrows indicate the scan direction and the position of the bulk material.

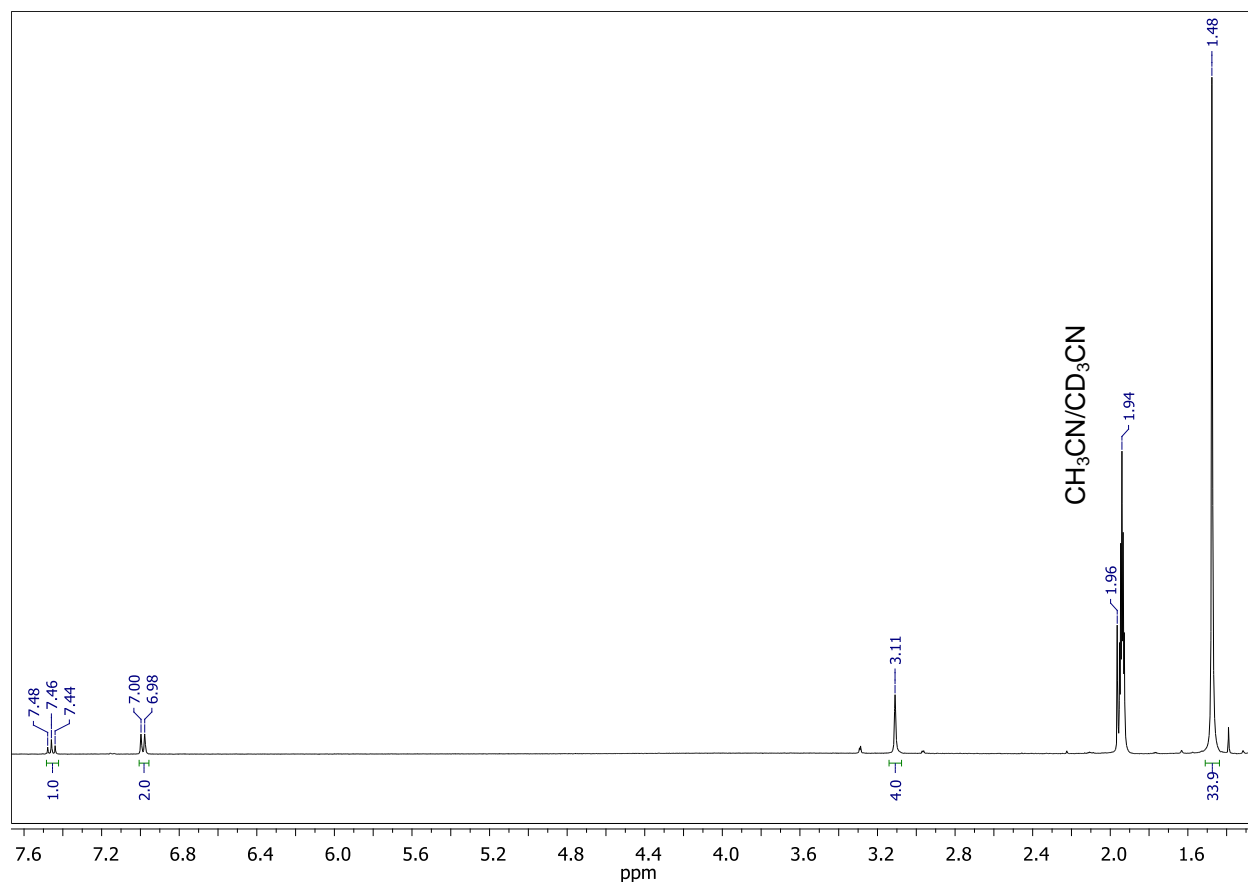


**Figure S5.** Cyclic voltammograms of 8 mM [HNEt<sub>3</sub>][BF<sub>4</sub>] alone in CH<sub>3</sub>CN with 0.20 M Bu<sub>4</sub>NPF<sub>6</sub> at a glassy carbon electrode (dotted black line) and with 1 mM [(P<sup>C</sup>N<sup>C</sup>P)Co(NCCH<sub>3</sub>)<sub>2</sub>][BF<sub>4</sub>]<sub>2</sub> (**1a**) under 1 atm CO<sub>2</sub> (solid red line).

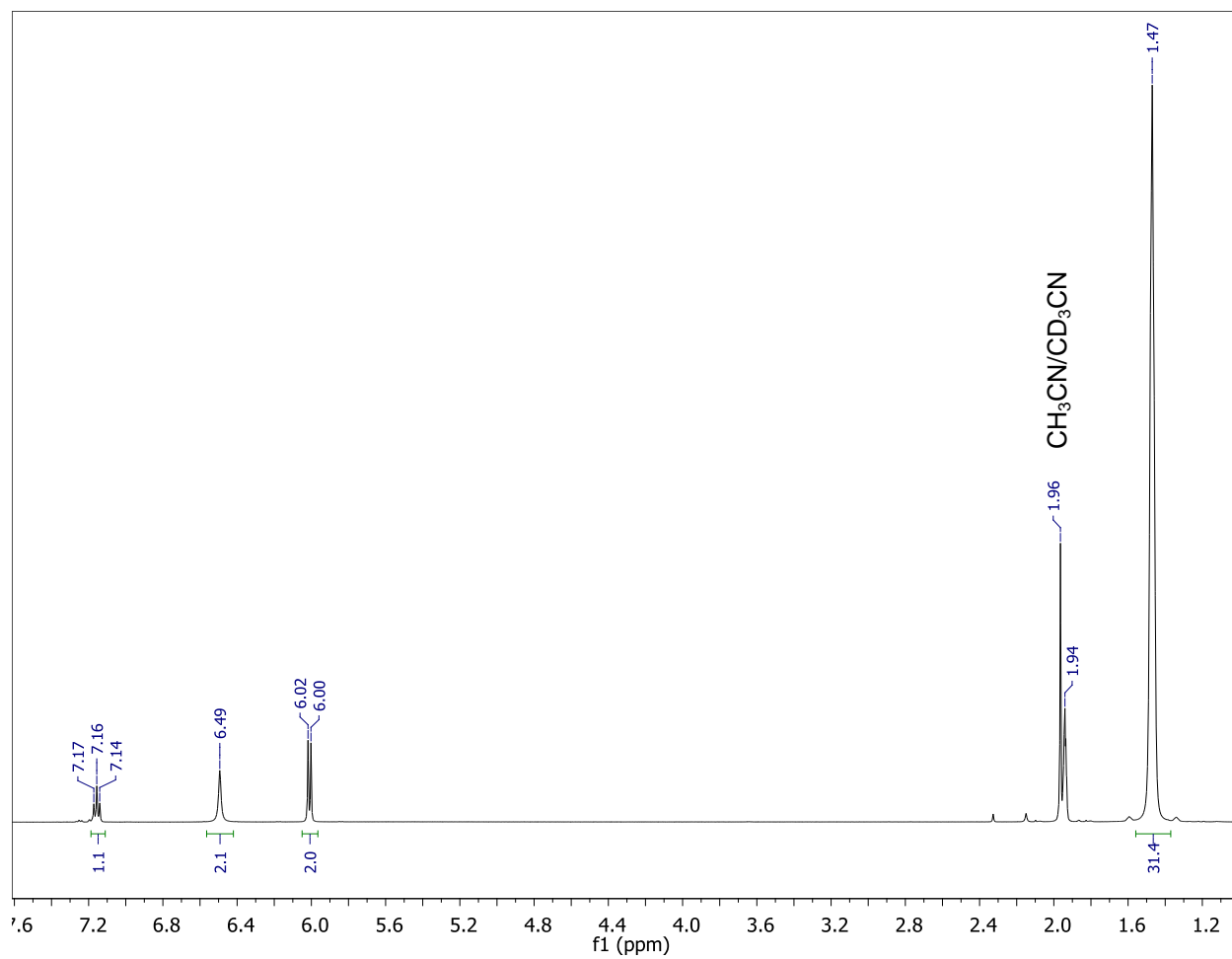
**Isolation of Proposed [(P<sup>C</sup>N<sup>C</sup>P)Co(CO)][BF<sub>4</sub>].** A dark orange solution of **1a** (108.3 mg, 152.5 μmol) in 4 mL THF and 1 mL CH<sub>3</sub>CN was frozen, and then solid KC<sub>8</sub> (22.0 mg, 161.1 μmol) was added to the just-thawed solution. After stirring 1.5 h, 5 mL diethyl ether was added to the dark green solution to promote precipitation of KBF<sub>4</sub> and the suspension was filtered. The resulting solution of **2a** was freeze-pump-thawed two times, then stirred under 1 atm CO for 1 h, resulting in an orange solution. Removal of the solvent *in vacuo* provided a brown solid, which was washed with diethyl ether, filtered, and dried *in vacuo* (yield 82.0 mg). <sup>1</sup>H NMR (CD<sub>3</sub>CN) δ/ppm: 7.87 (t, <sup>3</sup>J<sub>HH</sub> = 7.8 Hz, 1H, aryl-H), 7.49 (d, <sup>3</sup>J<sub>HH</sub> = 7.8 Hz, 2H, aryl-H), 3.85 (vt, 4H, -CH<sub>2</sub>-) 1.43 (vt, 36H, <sup>t</sup>Bu). <sup>13</sup>C{<sup>1</sup>H} NMR (126 MHz, CD<sub>3</sub>CN) δ/ppm: 166.8 (t, <sup>2</sup>J<sub>CP</sub> = 7.2 Hz), 141.9, 122.4 (t, <sup>3</sup>J<sub>CP</sub> = 5.3 Hz), 36.6 (t, <sup>1</sup>J<sub>CP</sub> = 9.8 Hz), 35.1 (t, <sup>2</sup>J<sub>CP</sub> = 8.3 Hz), 29.4 (br t). <sup>31</sup>P{<sup>1</sup>H} NMR (162 MHz, CD<sub>3</sub>CN) δ/ppm: 86.5 (br s, P<sup>t</sup>Bu<sub>2</sub>). IR (solid)  $\bar{\nu}_{\max}/\text{cm}^{-1}$ : 1918 (C≡O), 1875 (weak). IR (CH<sub>3</sub>CN with 0.20 M Bu<sub>4</sub>NBF<sub>4</sub>)  $\bar{\nu}_{\max}/\text{cm}^{-1}$ : 1920 (C≡O).



**Figure S6.** Cyclic voltammograms of the first reduction of 1 mM [(P<sup>C</sup>N<sup>C</sup>P)Co(NCCH<sub>3</sub>)<sub>2</sub>][BF<sub>4</sub>]<sub>2</sub> (**1a**) in CH<sub>3</sub>CN with 0.20 M Bu<sub>4</sub>NPF<sub>6</sub> upon sequential addition of increasingly strong acids.

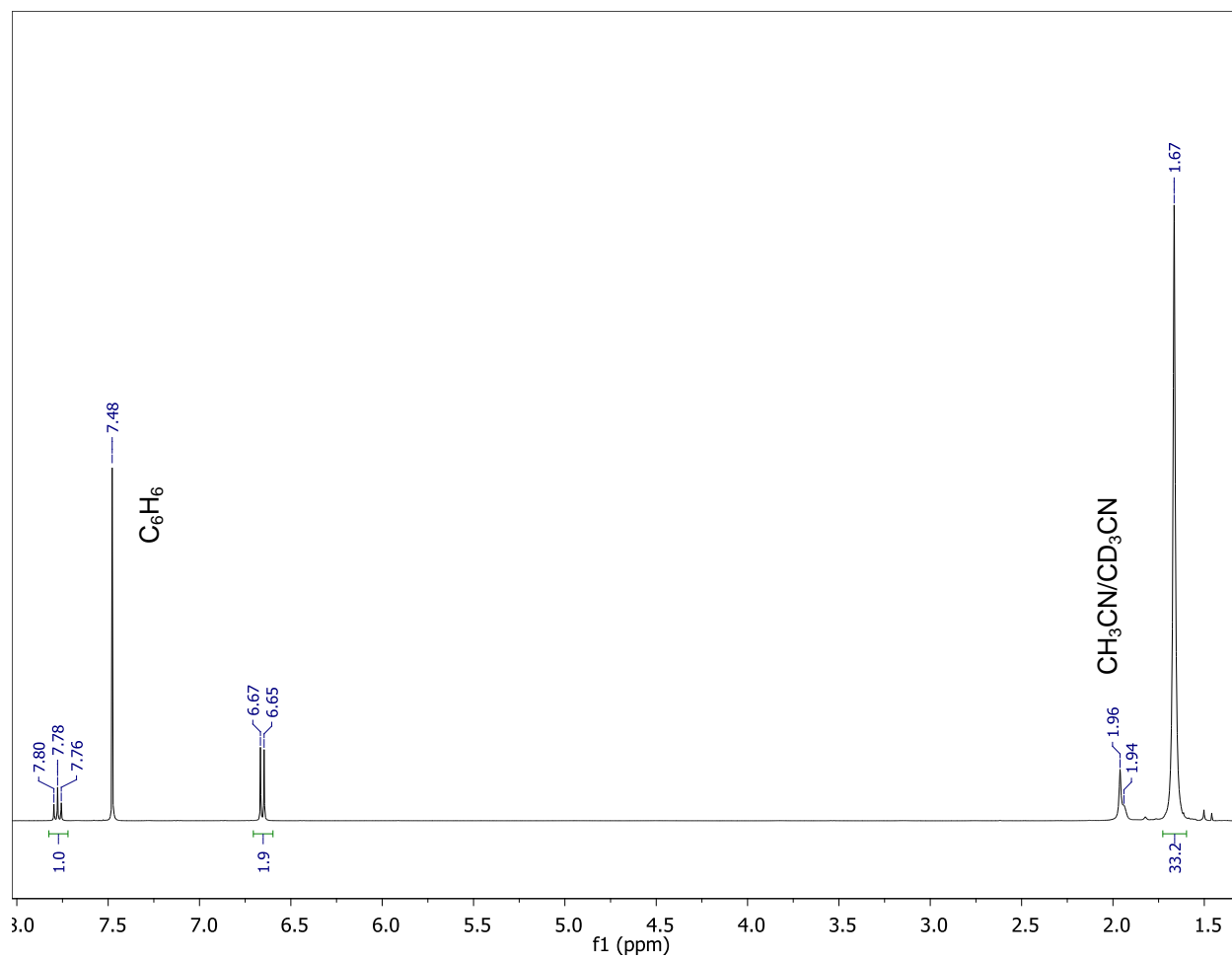


**Figure S7.**  $^1\text{H}$  NMR spectrum of  $[(\text{P}^{\text{C}}\text{N}^{\text{C}}\text{P})\text{Co}(\text{NCCH}_3)][\text{BF}_4]$  (**2a**) in  $\text{CD}_3\text{CN}$ .

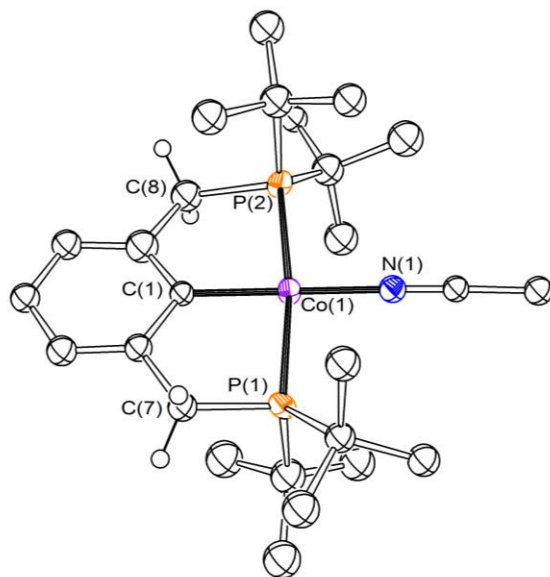


**Figure S8.**  $^1\text{H}$  NMR spectrum of  $[(\text{P}^{\text{N}}\text{N}^{\text{N}}\text{P})\text{Co}(\text{NCCH}_3)][\text{BF}_4]$  (**2b**) in  $\text{CD}_3\text{CN}$ .

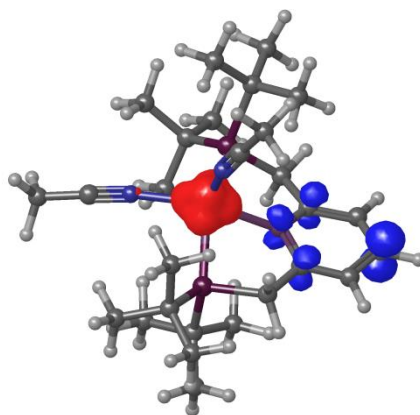




**Figure S9.**  $^1\text{H}$  NMR spectrum of  $[(\text{P}^{\text{O}}\text{N}^{\text{O}}\text{P})\text{Co}(\text{NCCH}_3)][\text{BF}_4]$  (**2c**) in  $\text{CD}_3\text{CN}$ .

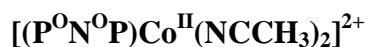


**Figure S10.** ORTEP diagram of one of four  $[(P^C N^C P)Co(NCCH_3)] [BF_4]$  (**2a**) molecules in the asymmetric unit from a low-quality X-ray structure. Isotropic thermal parameters were used in the refinement. Hydrogen atoms (except  $-CH_2-$ ) and outer-sphere  $BF_4$  anion have been omitted for clarity.



**Figure S11.** Spin density plot of  $[(P^C N^C P)Co(NCCH_3)_2]^0$ . Two upward spins on the metal are paired with a downward spin on the pyridine ring, creating a broken-symmetry doublet.

**Table S2.** Calculated geometries of Co complexes by DFT.



|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 0.0206010840  | -0.4072855773 | 0.4305195880  |
| P2  | 2.3896482356  | 0.0672460155  | -0.0742127940 |
| P3  | -2.3915377247 | -0.0103172265 | -0.0471068333 |
| O4  | 2.2620141943  | 1.7295219219  | -0.3412636568 |
| C5  | 1.0955656002  | 2.3922093847  | -0.1746459589 |
| C6  | 1.1121040310  | 3.7797071810  | -0.2550261115 |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| H7  | 2.0494834575  | 4.2918288611  | -0.4325244585 |
| C8  | -0.0995895856 | 4.4537692820  | -0.1114525256 |
| H9  | -0.1230058043 | 5.5376159611  | -0.1679333157 |
| C10 | -1.2855891172 | 3.7448612562  | 0.0812043267  |
| H11 | -2.2504453223 | 4.2290365862  | 0.1653523766  |
| C12 | -1.2093471552 | 2.3593141862  | 0.1309940741  |
| N13 | -0.0381625315 | 1.6815482552  | 0.0397121063  |
| O14 | -2.3578588572 | 1.6546048597  | 0.2580889289  |
| C15 | 3.7026905322  | 0.0182026690  | 1.2625697291  |
| C16 | 3.3188775431  | 1.1044898571  | 2.2947257205  |
| H17 | 2.2812129984  | 1.0188723689  | 2.6281392288  |
| H18 | 3.4676651439  | 2.1092821852  | 1.8922953685  |
| H19 | 3.9632782561  | 0.9953921188  | 3.1734988578  |
| C20 | 5.1353293299  | 0.2916292193  | 0.7705898136  |
| H21 | 5.8016721143  | 0.3299450341  | 1.6393784050  |
| H22 | 5.2127983112  | 1.2515987633  | 0.2536670772  |
| H23 | 5.5086737493  | -0.4957758272 | 0.1122213813  |
| C24 | 3.6094707135  | -1.3809736906 | 1.9111672312  |
| H25 | 3.8521970598  | -2.1829469038 | 1.2077170715  |
| H26 | 2.6129832940  | -1.5731969924 | 2.3231521701  |
| H27 | 4.3309581953  | -1.4418206719 | 2.7327039050  |
| C28 | 2.9719014816  | -0.4873013938 | -1.7668509385 |
| C29 | 4.0614719490  | 0.4136371694  | -2.3838756566 |
| H30 | 5.0249721023  | 0.3127350702  | -1.8861218617 |
| H31 | 3.7704192083  | 1.4671335271  | -2.3697872260 |
| H32 | 4.2025789964  | 0.1216842155  | -3.4304264410 |
| C33 | 3.4458089304  | -1.9516857770 | -1.6713205987 |
| H34 | 3.6437637556  | -2.3267785408 | -2.6811943059 |
| H35 | 2.6875272257  | -2.6021305411 | -1.2199631680 |
| H36 | 4.3720225683  | -2.0520099345 | -1.1004769866 |
| C37 | 1.7116674040  | -0.4092372607 | -2.6592919384 |
| H38 | 1.9536285964  | -0.7642890907 | -3.6666378793 |
| H39 | 1.3516116097  | 0.6197577431  | -2.7561396502 |
| H40 | 0.8949875946  | -1.0375647325 | -2.2814620696 |
| C41 | -3.8076875307 | -0.4712426425 | 1.0933238025  |
| C42 | -3.2233369506 | -0.4662508450 | 2.5233877042  |
| H43 | -4.0274083920 | -0.6840786089 | 3.2340396880  |
| H44 | -2.8062994045 | 0.5122273000  | 2.7838352729  |
| H45 | -2.4499504295 | -1.2290771074 | 2.6470935463  |
| C46 | -4.2755515002 | -1.8988501057 | 0.7438445367  |
| H47 | -3.4471796491 | -2.6176087083 | 0.7388413310  |
| H48 | -4.7849859996 | -1.9464071773 | -0.2210277053 |
| H49 | -4.9894264129 | -2.2312287901 | 1.5045917869  |
| C50 | -4.9839672364 | 0.5270421858  | 1.0410091192  |
| H51 | -5.5103312921 | 0.5170420306  | 0.0880856268  |
| H52 | -4.6563942076 | 1.5486686513  | 1.2469995843  |

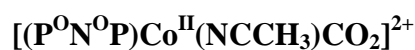
|     |               |               |               |
|-----|---------------|---------------|---------------|
| H53 | -5.7066478163 | 0.2449726164  | 1.8145478629  |
| C54 | -2.8429825644 | -0.0962752868 | -1.8763993911 |
| C55 | -2.5400289352 | -1.5406308134 | -2.3371355520 |
| H56 | -2.7389964355 | -1.6191556099 | -3.4113130005 |
| H57 | -3.1650147435 | -2.2837131799 | -1.8346091548 |
| H58 | -1.4895181491 | -1.8068533575 | -2.1760335546 |
| C59 | -4.2949373086 | 0.2860034781  | -2.2135890039 |
| H60 | -4.5448353988 | 1.2874138273  | -1.8534652825 |
| H61 | -5.0210522521 | -0.4249143384 | -1.8147026068 |
| H62 | -4.4113405253 | 0.2895051719  | -3.3031340465 |
| C63 | -1.8980611117 | 0.8764084023  | -2.6191396037 |
| H64 | -0.8447696639 | 0.6926026085  | -2.3944043555 |
| H65 | -2.1251451519 | 1.9210630851  | -2.3895375991 |
| H66 | -2.0314317547 | 0.7411249714  | -3.6975956471 |
| N67 | 0.0535021597  | -2.4890803086 | 0.0840087338  |
| C69 | 0.0533563276  | -3.6262419631 | -0.1371315665 |
| C72 | 0.0542406698  | -5.0542936887 | -0.4142220898 |
| H73 | 0.6287949262  | -5.5783993100 | 0.3562936864  |
| H74 | -0.9720570111 | -5.4343472486 | -0.4198916504 |
| H75 | 0.5130234849  | -5.2396432724 | -1.3907458150 |
| N73 | 0.0394480404  | -0.3065160073 | 2.5021742312  |
| C75 | 0.0205029274  | -0.1384845356 | 3.6472377179  |
| C78 | -0.0096209239 | 0.0895903138  | 5.0822261588  |
| H79 | 0.4185580497  | 1.0724409324  | 5.3047009120  |
| H80 | -1.0435169908 | 0.0571184881  | 5.4399894701  |
| H81 | 0.5756216151  | -0.6803345190 | 5.5945789101  |

**$[(P^ON^OP)Co^{II}(NCCH_3)]^+$**

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 0.0092357802  | -0.2587100406 | -0.0849492230 |
| P2  | 2.2607434466  | 0.0466679877  | -0.0579147072 |
| P3  | -2.2459006139 | 0.0135731397  | -0.1172061381 |
| O4  | 2.3143210049  | 1.7244663617  | -0.1407184324 |
| C5  | 1.1552846259  | 2.4109873102  | -0.1097836616 |
| C6  | 1.1888905913  | 3.7973049483  | -0.1085876812 |
| H7  | 2.1454926559  | 4.3040048969  | -0.1296713210 |
| C8  | -0.0257845150 | 4.4808066388  | -0.0781574404 |
| H9  | -0.0338821982 | 5.5662422697  | -0.0758473103 |
| C10 | -1.2301947670 | 3.7791065130  | -0.0507586280 |
| H11 | -2.1942990295 | 4.2713768493  | -0.0277345640 |
| C12 | -1.1759041658 | 2.3935796785  | -0.0547160548 |
| N13 | -0.0050571139 | 1.6946110441  | -0.0833352841 |
| O14 | -2.3247092065 | 1.6898100549  | -0.0260614915 |
| C15 | 3.1090349776  | -0.2827290899 | 1.5665299190  |
| C16 | 2.3141719093  | 0.5439693533  | 2.6069499908  |
| H17 | 1.2453458692  | 0.2921440716  | 2.6086685962  |
| H18 | 2.4197527384  | 1.6198532699  | 2.4452968675  |

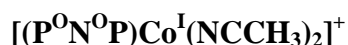
|     |               |               |               |
|-----|---------------|---------------|---------------|
| H19 | 2.7018531169  | 0.3186928875  | 3.6053766364  |
| C20 | 4.5865583074  | 0.1518109060  | 1.5612222581  |
| H21 | 4.9783880770  | 0.0748530097  | 2.5810487848  |
| H22 | 4.7084347702  | 1.1886806432  | 1.2360247158  |
| H23 | 5.1999778347  | -0.4928178837 | 0.9270691034  |
| C24 | 2.9731998828  | -1.7843095799 | 1.8984153808  |
| H25 | 3.4919467356  | -2.4235964863 | 1.1802341484  |
| H26 | 1.9246257579  | -2.0951836173 | 1.9544714218  |
| H27 | 3.4227835632  | -1.9645448475 | 2.8802613135  |
| C28 | 3.1525139620  | -0.3985683965 | -1.6325460349 |
| C29 | 4.4017074979  | 0.4753416910  | -1.8708843715 |
| H30 | 5.1866373508  | 0.2939708817  | -1.1357243747 |
| H31 | 4.1608687296  | 1.5408542063  | -1.8674628221 |
| H32 | 4.8102100986  | 0.2275631917  | -2.8565407040 |
| C33 | 3.5232695471  | -1.8941725233 | -1.6098375851 |
| H34 | 3.8940496792  | -2.1782672528 | -2.6000246928 |
| H35 | 2.6625902232  | -2.5345564329 | -1.3858337117 |
| H36 | 4.3181490174  | -2.1079349536 | -0.8909055430 |
| C37 | 2.1136580803  | -0.1261982294 | -2.7489321088 |
| H38 | 2.5612210088  | -0.3540339960 | -3.7217598936 |
| H39 | 1.8025850452  | 0.9236088452  | -2.7720656890 |
| H40 | 1.2216112797  | -0.7584454576 | -2.6457882326 |
| C41 | -3.1370540883 | -0.4524455098 | 1.4514871335  |
| C42 | -2.1068480212 | -0.1688026944 | 2.5729519183  |
| H43 | -2.5553185740 | -0.4061222888 | 3.5431038395  |
| H44 | -1.8112436713 | 0.8853927797  | 2.6004875105  |
| H45 | -1.2052130112 | -0.7875643649 | 2.4714798908  |
| C46 | -3.4851796686 | -1.9534324962 | 1.4211741497  |
| H47 | -2.6133724816 | -2.5797557624 | 1.2005400254  |
| H48 | -4.2722834830 | -2.1764860732 | 0.6965286150  |
| H49 | -3.8575200296 | -2.2468147075 | 2.4080869602  |
| C50 | -4.4005747905 | 0.4014324972  | 1.6878878372  |
| H51 | -5.1795669089 | 0.2108380532  | 0.9487251730  |
| H52 | -4.1760657229 | 1.4705369493  | 1.6894563583  |
| H53 | -4.8092696552 | 0.1436679015  | 2.6708957339  |
| C54 | -3.0824316143 | -0.3208962075 | -1.7467496699 |
| C55 | -2.9234064880 | -1.8186914673 | -2.0848156226 |
| H56 | -3.3629978103 | -2.0003623299 | -3.0709179353 |
| H57 | -3.4391822280 | -2.4683056726 | -1.3737177752 |
| H58 | -1.8705636508 | -2.1157758660 | -2.1341350373 |
| C59 | -4.5659196487 | 0.0924099217  | -1.7455862550 |
| H60 | -4.7035966837 | 1.1266576025  | -1.4184391354 |
| H61 | -5.1721276984 | -0.5623435654 | -1.1149080221 |
| H62 | -4.9534021086 | 0.0122848470  | -2.7668445713 |
| C63 | -2.2955747198 | 0.5220027225  | -2.7801840964 |
| H64 | -1.2231865677 | 0.2861764230  | -2.7787699116 |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| H65 | -2.4177933339 | 1.5954500795  | -2.6143291186 |
| H66 | -2.6757946268 | 0.2954427867  | -3.7811542097 |
| N67 | 0.0200435946  | -2.1697699086 | -0.0757886326 |
| C69 | 0.0225554784  | -3.3272120623 | -0.0624066192 |
| C72 | 0.0262815241  | -4.7811065426 | -0.0451577783 |
| H73 | 0.6303808603  | -5.1387236840 | 0.7953629939  |
| H74 | -0.9966487745 | -5.1568890863 | 0.0605016803  |
| H75 | 0.4534883513  | -5.1595677102 | -0.9798384041 |



|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.3337171938  | 0.8951939914  | 0.3037610073  |
| N2  | 1.5519985455  | 0.8373474397  | -0.5168213504 |
| C3  | 0.8409783049  | 1.9734545089  | -0.7463274452 |
| C4  | -0.3811112787 | 1.9747504570  | -1.4052297970 |
| C5  | -0.8923591510 | 0.7527437489  | -1.8373558498 |
| C6  | -0.2001993074 | -0.4319978184 | -1.5846719465 |
| C7  | 1.0060636639  | -0.3460184046 | -0.9071132954 |
| H8  | -0.8969942971 | 2.9137245556  | -1.5612449593 |
| H9  | -1.8442619424 | 0.7202029397  | -2.3577531407 |
| H10 | -0.5794095162 | -1.4049968584 | -1.8707105449 |
| O11 | 1.3463454008  | 3.1394531525  | -0.2971820828 |
| O12 | 1.6690335680  | -1.4800049577 | -0.5882666260 |
| P17 | 2.9185303153  | 3.1751867679  | 0.3008032125  |
| P18 | 2.8856178164  | -1.3912250506 | 0.5712545708  |
| C19 | 1.9957836002  | -1.6899583436 | 2.2090053556  |
| C20 | 3.9379995225  | -2.8491335762 | 0.0266581367  |
| C21 | 2.6377665967  | 3.8945082066  | 2.0087832600  |
| C22 | 3.7584948099  | 4.3252243284  | -0.9110073287 |
| C25 | 3.3336050302  | 3.8583421336  | -2.3240064889 |
| H26 | 3.4953428519  | 2.7910156289  | -2.4859208076 |
| H27 | 2.2809771170  | 4.0792723053  | -2.5168000761 |
| H28 | 3.9278311513  | 4.4064847239  | -3.0622734123 |
| C29 | 3.3447370393  | 5.8003948242  | -0.7412734190 |
| H30 | 2.2612990512  | 5.9334368339  | -0.7988659217 |
| H31 | 3.7083874389  | 6.2336580851  | 0.1924666099  |
| H32 | 3.7903624125  | 6.3757689615  | -1.5599441995 |
| C33 | 5.2841308886  | 4.1716138586  | -0.7221404367 |
| H34 | 5.7917759254  | 4.7932363797  | -1.4668320759 |
| H35 | 5.6183697834  | 4.5108717338  | 0.2616125815  |
| H36 | 5.6160504935  | 3.1397890117  | -0.8625598141 |
| C37 | 1.6247137541  | 5.0602490455  | 2.0103941973  |
| H38 | 2.0113303862  | 5.9611577942  | 1.5368084723  |
| H39 | 0.6851023559  | 4.7845916291  | 1.5250187674  |
| H40 | 1.3991762206  | 5.3109566428  | 3.0527746914  |
| C41 | 2.0498591857  | 2.7405235242  | 2.8511405840  |
| H42 | 1.0808818965  | 2.4108651996  | 2.4641263406  |

|     |              |               |               |
|-----|--------------|---------------|---------------|
| H43 | 2.7259915513 | 1.8798113077  | 2.9057719509  |
| H44 | 1.8878585594 | 3.0879190435  | 3.8768172322  |
| C45 | 3.9922681196 | 4.3323572629  | 2.6033038801  |
| H46 | 3.8392105338 | 4.6161660306  | 3.6498081936  |
| H47 | 4.7357121733 | 3.5278773848  | 2.5881112438  |
| H48 | 4.4088772261 | 5.2020439619  | 2.0907904422  |
| C49 | 4.7633984180 | -2.3971680338 | -1.1963848986 |
| H50 | 4.1275683296 | -2.0126967060 | -1.9996468074 |
| H51 | 5.5008932832 | -1.6369061653 | -0.9290718804 |
| H52 | 5.3056199943 | -3.2643327899 | -1.5868693915 |
| C53 | 3.0613021909 | -4.0526195854 | -0.3930878071 |
| H54 | 2.3779785543 | -3.7948951572 | -1.2049965950 |
| H55 | 3.7308714999 | -4.8397148254 | -0.7561698432 |
| H56 | 2.4843175503 | -4.4733804353 | 0.4283212841  |
| C57 | 4.9020401789 | -3.2474974077 | 1.1637507540  |
| H58 | 5.5837565311 | -4.0150790304 | 0.7839664526  |
| H59 | 5.5250961000 | -2.4140864940 | 1.5061225953  |
| H60 | 4.3867622646 | -3.6739292289 | 2.0258134386  |
| C61 | 1.5088412732 | -3.1350775256 | 2.4279545602  |
| H62 | 0.8402721118 | -3.4641830261 | 1.6282737846  |
| H63 | 2.3259801601 | -3.8511816169 | 2.5255920928  |
| H64 | 0.9398526464 | -3.1662261695 | 3.3636866888  |
| C65 | 0.7609458691 | -0.7594860776 | 2.2409258124  |
| H66 | 0.0049805260 | -1.0590447512 | 1.5099736909  |
| H67 | 0.3009598441 | -0.8251088604 | 3.2322750508  |
| H68 | 1.0165183903 | 0.2875424399  | 2.0682099352  |
| C69 | 2.9765011153 | -1.2720352780 | 3.3296254418  |
| H70 | 2.4738916849 | -1.3757319265 | 4.2968783804  |
| H71 | 3.8740830023 | -1.8944053964 | 3.3654877668  |
| H72 | 3.2783172198 | -0.2228795718 | 3.2375086993  |
| N84 | 4.5792893671 | 0.7864905049  | -1.3870023010 |
| C85 | 5.2155932405 | 0.7320621873  | -2.3530241642 |
| C86 | 6.0091364566 | 0.6584479393  | -3.5704733583 |
| H87 | 5.6965646543 | 1.4450190481  | -4.2643872176 |
| H88 | 7.0690935379 | 0.7910295966  | -3.3327525644 |
| H89 | 5.8677788015 | -0.3170105489 | -4.0463765089 |
| C83 | 5.8783668385 | 0.3883391309  | 2.0242513990  |
| O84 | 5.0219769772 | 1.0624570561  | 1.5678092940  |
| O85 | 6.7145893985 | -0.2650281543 | 2.4796108759  |



|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 0.0185481878  | -0.6507420386 | -0.0505383785 |
| P2  | 2.3385947488  | 0.0271407812  | 0.0997914048  |
| P3  | -2.3168473893 | -0.0265803407 | 0.0276181698  |
| O4  | 2.3056760999  | 1.7081494349  | -0.1606541350 |
| C5  | 1.1335016808  | 2.3697870727  | -0.2910357802 |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| C6  | 1.1770341855  | 3.7591724094  | -0.4052932217 |
| H7  | 2.1328886861  | 4.2679477814  | -0.4009713264 |
| C8  | -0.0380583168 | 4.4332012380  | -0.5063205398 |
| H9  | -0.0509451030 | 5.5156023603  | -0.5916293542 |
| C10 | -1.2373269642 | 3.7243719228  | -0.4802092153 |
| H11 | -2.2058899981 | 4.2052945505  | -0.5352453893 |
| C12 | -1.1607733019 | 2.3371620420  | -0.3607464884 |
| N13 | -0.0048839739 | 1.6596498787  | -0.2888635763 |
| O14 | -2.3191159775 | 1.6418105584  | -0.2991039125 |
| C15 | 3.1143334175  | 0.0752689235  | 1.8176235240  |
| C16 | 1.9463092068  | 0.5079193149  | 2.7375040881  |
| H17 | 1.0975039991  | -0.1783298800 | 2.6692172331  |
| H18 | 1.5923716200  | 1.5153189066  | 2.4936207898  |
| H19 | 2.2879721854  | 0.5231233338  | 3.7789388030  |
| C20 | 4.2675560598  | 1.0804258795  | 2.0021658020  |
| H21 | 4.4902827950  | 1.1727532371  | 3.0719868296  |
| H22 | 3.9990266763  | 2.0723469532  | 1.6298498669  |
| H23 | 5.1852737929  | 0.7636168544  | 1.5068037657  |
| C24 | 3.5657816228  | -1.3476430223 | 2.1964813237  |
| H25 | 4.4468438545  | -1.6597966443 | 1.6280641135  |
| H26 | 2.7712619493  | -2.0849455772 | 2.0351716925  |
| H27 | 3.8370713539  | -1.3727320611 | 3.2584615283  |
| C28 | 3.5695411494  | -0.3855610711 | -1.2617509198 |
| C29 | 4.9727238167  | 0.2199052680  | -1.0897369402 |
| H30 | 5.5318855236  | -0.2591487246 | -0.2822439556 |
| H31 | 4.9278558267  | 1.2951065466  | -0.8963431198 |
| H32 | 5.5438232520  | 0.0705514617  | -2.0139404084 |
| C33 | 3.6573738697  | -1.9216641543 | -1.3696583868 |
| H34 | 4.2773228400  | -2.1871266071 | -2.2340151293 |
| H35 | 2.6712691208  | -2.3754340303 | -1.5047258495 |
| H36 | 4.1209305991  | -2.3715077615 | -0.4868710919 |
| C37 | 2.9460367705  | 0.1914655710  | -2.5569677883 |
| H38 | 3.5223535007  | -0.1645494121 | -3.4186677258 |
| H39 | 2.9799441028  | 1.2839888433  | -2.5599620913 |
| H40 | 1.9062582054  | -0.1165310401 | -2.6911119071 |
| C41 | -3.1396995465 | 0.0586796823  | 1.7249584719  |
| C42 | -1.9901022169 | 0.4606147538  | 2.6811371095  |
| H43 | -2.3718719688 | 0.5231700156  | 3.7068253653  |
| H44 | -1.5746812779 | 1.4413785178  | 2.4258265223  |
| H45 | -1.1752968414 | -0.2678505917 | 2.6667686962  |
| C46 | -3.6533022763 | -1.3434987049 | 2.1033667986  |
| H47 | -2.8864004053 | -2.1131528327 | 1.9586757775  |
| H48 | -4.5358237965 | -1.6251483565 | 1.5220387660  |
| H49 | -3.9422605995 | -1.3525382845 | 3.1609638723  |
| C50 | -4.2625956408 | 1.1051258296  | 1.8631680787  |
| H51 | -5.1596086741 | 0.8407000111  | 1.3038333330  |



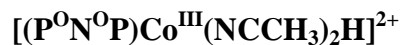
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|-----|---------------|---------------|---------------|
| H52 | -3.9313696832 | 2.0927717384  | 1.5331669010  |
| H53 | -4.5467530342 | 1.1821399522  | 2.9196163529  |
| C54 | -3.5072229258 | -0.5317606937 | -1.3371023384 |
| C55 | -3.5164866206 | -2.0733909936 | -1.3977276992 |
| H56 | -4.1175705932 | -2.3967293670 | -2.2556005384 |
| H57 | -3.9593194165 | -2.5202850769 | -0.5029766347 |
| H58 | -2.5068468556 | -2.4776135299 | -1.5166941761 |
| C59 | -4.9396155939 | 0.0095689247  | -1.1988093935 |
| H60 | -4.9488651126 | 1.0949865879  | -1.0673082858 |
| H61 | -5.4767353617 | -0.4497772241 | -0.3650775708 |
| H62 | -5.5004067045 | -0.2202585398 | -2.1126884793 |
| C63 | -2.8944480915 | 0.0318097735  | -2.6424964271 |
| H64 | -1.8424867030 | -0.2413840063 | -2.7569927064 |
| H65 | -2.9690915826 | 1.1215356763  | -2.6774954218 |
| H66 | -3.4477301385 | -0.3716242579 | -3.4983917938 |
| N67 | 0.0707389537  | -1.6710740852 | -1.8253586183 |
| C69 | 0.1262831622  | -2.2399577041 | -2.8354645535 |
| C72 | 0.2078656232  | -2.9399039248 | -4.1111769885 |
| H73 | 0.3341285452  | -4.0137005197 | -3.9436603577 |
| H74 | -0.7066650429 | -2.7753495138 | -4.6892366958 |
| H75 | 1.0622027283  | -2.5676663787 | -4.6852150881 |
| N73 | -0.0149396058 | -2.2608010375 | 1.2710909607  |
| C75 | -0.0805579517 | -2.9928186702 | 2.1699985013  |
| C78 | -0.1786693039 | -3.9074162191 | 3.3001686929  |
| H79 | 0.2307056421  | -3.4358242534 | 4.1986225703  |
| H80 | -1.2259571560 | -4.1675264224 | 3.4819703114  |
| H81 | 0.3836745100  | -4.8225186273 | 3.0930218153  |

$[(P^O N^O P)Co^I(NCCH_3)]^+$

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 0.0051532315  | -0.4924560205 | -0.0864003737 |
| P2  | 2.2636610107  | 0.0621620475  | -0.0527373267 |
| P3  | -2.2603904520 | 0.0298400444  | -0.1067228635 |
| O4  | 2.2977299487  | 1.7620455262  | -0.1239477870 |
| C5  | 1.1379168617  | 2.4652144184  | -0.1017681052 |
| C6  | 1.1872052492  | 3.8574932408  | -0.1007598497 |
| H7  | 2.1427522042  | 4.3665754255  | -0.1167376102 |
| C8  | -0.0304101403 | 4.5383035120  | -0.0782700441 |
| H9  | -0.0379973940 | 5.6240425484  | -0.0763148712 |
| C10 | -1.2384608156 | 3.8405300845  | -0.0580089878 |
| H11 | -2.2010704821 | 4.3360373561  | -0.0395363961 |
| C12 | -1.1694706809 | 2.4490273561  | -0.0617936376 |
| N13 | -0.0110056206 | 1.7768792988  | -0.0833104797 |
| O14 | -2.3191968401 | 1.7293619662  | -0.0404366277 |
| C15 | 3.1899432502  | -0.1876435889 | 1.5565387882  |
| C16 | 2.3749213604  | 0.6078543152  | 2.6050130760  |
| H17 | 1.3146548706  | 0.3248576811  | 2.6012258050  |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| H18 | 2.4423125466  | 1.6861224610  | 2.4367814923  |
| H19 | 2.7710153875  | 0.3969256542  | 3.6044080005  |
| C20 | 4.6455325956  | 0.3040122190  | 1.5555720890  |
| H21 | 5.0469384170  | 0.2543912029  | 2.5744965430  |
| H22 | 4.7213052552  | 1.3404336196  | 1.2151751440  |
| H23 | 5.2843632710  | -0.3190616975 | 0.9240162610  |
| C24 | 3.1182705962  | -1.6892430124 | 1.9047680164  |
| H25 | 3.6752565009  | -2.3082988242 | 1.1961791589  |
| H26 | 2.0827471069  | -2.0456318884 | 1.9292000573  |
| H27 | 3.5552489991  | -1.8500308212 | 2.8967036600  |
| C28 | 3.2623624484  | -0.2741831028 | -1.6031723268 |
| C29 | 4.4824483666  | 0.6437824923  | -1.8049343022 |
| H30 | 5.2749329459  | 0.4515500637  | -1.0806003580 |
| H31 | 4.2051766907  | 1.6986131773  | -1.7395599235 |
| H32 | 4.8997047052  | 0.4658912933  | -2.8030580272 |
| C33 | 3.6834519575  | -1.7559150350 | -1.6135479071 |
| H34 | 4.0885359035  | -2.0095107289 | -2.5998146969 |
| H35 | 2.8362346185  | -2.4242409812 | -1.4202520053 |
| H36 | 4.4648759495  | -1.9623850535 | -0.8765224728 |
| C37 | 2.2509576806  | -0.0176796272 | -2.7481037955 |
| H38 | 2.7277650327  | -0.2235546299 | -3.7129239044 |
| H39 | 1.9133844638  | 1.0239526440  | -2.7607032825 |
| H40 | 1.3693085918  | -0.6660847370 | -2.6666325109 |
| C41 | -3.2388712298 | -0.3172924306 | 1.4544359504  |
| C42 | -2.2226463634 | -0.0338878491 | 2.5886703109  |
| H43 | -2.6864165806 | -0.2446553256 | 3.5587291513  |
| H44 | -1.9064892442 | 1.0144588168  | 2.5929881331  |
| H45 | -1.3284716306 | -0.6644119728 | 2.5027187035  |
| C46 | -3.6295016969 | -1.8071934324 | 1.4774811208  |
| H47 | -2.7703184616 | -2.4591188848 | 1.2807668695  |
| H48 | -4.4129681253 | -2.0339865167 | 0.7486826421  |
| H49 | -4.0204590679 | -2.0630117486 | 2.4688687025  |
| C50 | -4.4751603533 | 0.5772300871  | 1.6621473226  |
| H51 | -5.2709921955 | 0.3630466480  | 0.9476789786  |
| H52 | -4.2200559742 | 1.6369501386  | 1.5855354593  |
| H53 | -4.8782851229 | 0.3989688329  | 2.6659986400  |
| C54 | -3.1962245927 | -0.2367823356 | -1.7071523353 |
| C55 | -3.1147517870 | -1.7391945907 | -2.0493709823 |
| H56 | -3.5573728990 | -1.9077088415 | -3.0374864357 |
| H57 | -3.6621783426 | -2.3594307096 | -1.3343948603 |
| H58 | -2.0767989766 | -2.0877103714 | -2.0797380893 |
| C59 | -4.6556499541 | 0.2429798397  | -1.6971633239 |
| H60 | -4.7376938803 | 1.2791290933  | -1.3574463630 |
| H61 | -5.2848422919 | -0.3846222582 | -1.0604885236 |
| H62 | -5.0634280103 | 0.1886077969  | -2.7132895189 |
| C63 | -2.3950454399 | 0.5607062840  | -2.7647673859 |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| H64 | -1.3326833238 | 0.2856311559  | -2.7675317802 |
| H65 | -2.4693044814 | 1.6391209697  | -2.6003402684 |
| H66 | -2.7967047359 | 0.3427682124  | -3.7604138029 |
| N67 | 0.0157475609  | -2.5643541968 | -0.0973404145 |
| C69 | 0.0164059981  | -3.7252722475 | -0.1001832686 |
| C72 | 0.0175005899  | -5.1829854059 | -0.1026516370 |
| H73 | 0.5711977273  | -5.5564918426 | 0.7641563461  |
| H74 | -1.0079886157 | -5.5622137757 | -0.0605010356 |
| H75 | 0.4963449601  | -5.5528404768 | -1.0143205821 |



|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.3814401144  | 0.8398330307  | 0.9782101635  |
| N2  | 1.8526760858  | 0.9943230392  | -0.2360839800 |
| C3  | 1.3247236252  | 2.2118280111  | -0.5159404429 |
| C4  | 0.1794723223  | 2.3745332808  | -1.2810237475 |
| C5  | -0.4169615689 | 1.2287970463  | -1.8095054185 |
| C6  | 0.1371804735  | -0.0287822319 | -1.5791230429 |
| C7  | 1.2782403127  | -0.1006380383 | -0.7894464722 |
| H8  | -0.1969024756 | 3.3717096838  | -1.4712243741 |
| H9  | -1.3076484407 | 1.3199923952  | -2.4231636346 |
| H10 | -0.2802465913 | -0.9379628237 | -1.9932129019 |
| O11 | 1.9801049196  | 3.2959391868  | -0.0396432439 |
| O12 | 1.8577080798  | -1.2974077683 | -0.5652829271 |
| P17 | 3.5724136313  | 3.0619360734  | 0.4685527120  |
| P18 | 3.1681280214  | -1.3868872523 | 0.4877337929  |
| C19 | 2.5255636437  | -2.5372223637 | 1.8401253133  |
| C20 | 4.4482400033  | -2.1759650128 | -0.6439435238 |
| C21 | 3.7210359560  | 4.4316095002  | 1.7452368902  |
| C22 | 4.5843214071  | 3.4024637611  | -1.0920027931 |
| C23 | 3.9501279391  | 2.5974295238  | -2.2516699607 |
| H24 | 3.8691943672  | 1.5311507605  | -2.0361000913 |
| H25 | 2.9615773944  | 2.9797176867  | -2.5205030315 |
| H26 | 4.5899897826  | 2.7060212770  | -3.1333401465 |
| C27 | 4.6019650668  | 4.8865966691  | -1.5118087759 |
| H28 | 3.5934590100  | 5.2836450137  | -1.6542652755 |
| H29 | 5.1397027186  | 5.5230268390  | -0.8074975415 |
| H30 | 5.1216014222  | 4.9624045951  | -2.4729878108 |
| C31 | 6.0254036017  | 2.8997876729  | -0.8464145316 |
| H32 | 6.5956525136  | 3.0127151456  | -1.7744634523 |
| H33 | 6.5466839260  | 3.4707656662  | -0.0748419190 |
| H34 | 6.0524153468  | 1.8414897611  | -0.5704246485 |
| C35 | 3.0405799049  | 5.7398188116  | 1.2789324397  |
| H36 | 3.5398671319  | 6.2087928746  | 0.4336344150  |
| H37 | 1.9912276487  | 5.5807108950  | 1.0197045470  |
| H38 | 3.0746771628  | 6.4506402279  | 2.1116816862  |
| C39 | 3.0146731441  | 3.9558457417  | 3.0314151256  |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| H40 | 1.9517674038  | 3.7679295642  | 2.8565726373  |
| H41 | 3.4739692857  | 3.0546702941  | 3.4441927026  |
| H42 | 3.0918762418  | 4.7499664631  | 3.7808458406  |
| C43 | 5.2157000269  | 4.6627265265  | 2.0541305792  |
| H44 | 5.2929572536  | 5.3606029081  | 2.8940343691  |
| H45 | 5.7260568975  | 3.7386105427  | 2.3489742547  |
| H46 | 5.7558756738  | 5.1058938802  | 1.2160398413  |
| C47 | 4.8315037801  | -1.1540224402 | -1.7370512287 |
| H48 | 3.9610301460  | -0.8176026562 | -2.3092281366 |
| H49 | 5.3501647330  | -0.2816702344 | -1.3338119206 |
| H50 | 5.5141304349  | -1.6405406123 | -2.4411175051 |
| C51 | 3.8933115860  | -3.4288916704 | -1.3646514211 |
| H52 | 2.9421912456  | -3.2234046512 | -1.8632021273 |
| H53 | 4.6122636175  | -3.7205592316 | -2.1370723590 |
| H54 | 3.7683537255  | -4.2847320970 | -0.7066139068 |
| C55 | 5.6937078690  | -2.5160558336 | 0.2000150726  |
| H56 | 6.4712828948  | -2.9130990481 | -0.4610409793 |
| H57 | 6.1052378925  | -1.6278938580 | 0.6928312053  |
| H58 | 5.4938651313  | -3.2771577510 | 0.9583594879  |
| C59 | 2.6199698960  | -4.0456711337 | 1.5401389917  |
| H60 | 2.0634705518  | -4.3234626973 | 0.6426060491  |
| H61 | 3.6490430012  | -4.3978375889 | 1.4476666929  |
| H62 | 2.1701271272  | -4.5839303708 | 2.3816478510  |
| C63 | 1.0317342278  | -2.1925286707 | 2.0464533198  |
| H64 | 0.4266270785  | -2.5427955049 | 1.2070211304  |
| H65 | 0.6806010388  | -2.7028012916 | 2.9494149399  |
| H66 | 0.8517358387  | -1.1249414166 | 2.1715780077  |
| C67 | 3.3452789723  | -2.2141772948 | 3.1107328689  |
| H68 | 2.9784605321  | -2.8357950789 | 3.9339796137  |
| H69 | 4.4078602956  | -2.4445330991 | 2.9798904359  |
| H70 | 3.2528354660  | -1.1672107211 | 3.4072655529  |
| N71 | 4.9223496747  | 0.6974837248  | 2.1139305379  |
| C72 | 5.8627174246  | 0.5957260380  | 2.7773029999  |
| C73 | 7.0541936113  | 0.4637198208  | 3.6029518900  |
| H74 | 7.9256815326  | 0.2841241799  | 2.9654853044  |
| H75 | 7.2146039791  | 1.3813004907  | 4.1774736915  |
| H76 | 6.9364467672  | -0.3761552179 | 4.2945206854  |
| H77 | 4.2532964207  | 0.7407701932  | -0.1427046138 |
| N78 | 2.0872538424  | 0.9937746187  | 2.5570521711  |
| C79 | 0.3398120037  | 1.2796907509  | 4.4764645756  |
| C80 | 1.3142479213  | 1.1158315078  | 3.4085930624  |
| H81 | -0.6554598622 | 1.0024208178  | 4.1156768881  |
| H82 | 0.6041496502  | 0.6416851337  | 5.3251162768  |
| H83 | 0.3239268356  | 2.3240489475  | 4.8038407059  |



|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.5039596363  | 0.8594878721  | 0.2046057710  |
| N2  | 1.5303697961  | 0.8087349239  | -0.5362067700 |
| C3  | 0.7861767356  | 1.9221586897  | -0.5953513654 |
| C4  | -0.5048440022 | 1.9302985002  | -1.1194590182 |
| C5  | -1.0139592395 | 0.7175523046  | -1.5848218404 |
| C6  | -0.2684601255 | -0.4594680804 | -1.4852023103 |
| C7  | 0.9969883557  | -0.3623440736 | -0.9145964495 |
| H8  | -1.0723995358 | 2.8519136552  | -1.1443022441 |
| H9  | -2.0145682716 | 0.6829129066  | -2.0043031575 |
| H10 | -0.6524535516 | -1.4243643227 | -1.7911350559 |
| O11 | 1.3128413730  | 3.0698435402  | -0.1001133073 |
| O12 | 1.7184212677  | -1.4845641257 | -0.6678930454 |
| P17 | 2.9737542564  | 3.1314773016  | 0.2980079323  |
| P18 | 2.9396551030  | -1.4155173842 | 0.5354872930  |
| C19 | 1.9031079759  | -1.8246868137 | 2.0715626087  |
| C20 | 3.9269348591  | -2.9196001216 | -0.0469368815 |
| C21 | 2.8504431114  | 4.0165918740  | 1.9544792309  |
| C22 | 3.5432746549  | 4.2775161597  | -1.0855410167 |
| C25 | 3.0451046659  | 3.6163156815  | -2.3945006510 |
| H26 | 3.3185963222  | 2.5614471584  | -2.4598886380 |
| H27 | 1.9591181671  | 3.6943045208  | -2.4910904479 |
| H28 | 3.4925271442  | 4.1383121708  | -3.2477173088 |
| C29 | 2.9770764755  | 5.7060780024  | -1.0232910363 |
| H30 | 1.8863551665  | 5.7033746303  | -0.9452743871 |
| H31 | 3.3880503748  | 6.2816044898  | -0.1903194738 |
| H32 | 3.2434197452  | 6.2355397319  | -1.9457978862 |
| C33 | 5.0865123178  | 4.3098255323  | -1.0785103268 |
| H34 | 5.4367208544  | 4.8497062336  | -1.9660797299 |
| H35 | 5.4878691115  | 4.8291304051  | -0.2047811379 |
| H36 | 5.5144200474  | 3.3041236911  | -1.1011207638 |
| C37 | 1.7646414169  | 5.1076716764  | 2.0359482925  |
| H38 | 1.9880571134  | 5.9743028142  | 1.4143041884  |
| H39 | 0.7860148069  | 4.7184412662  | 1.7445019638  |
| H40 | 1.6937453432  | 5.4583338547  | 3.0724066873  |
| C41 | 2.4998081886  | 2.9133444609  | 2.9794365423  |
| H42 | 1.5123064201  | 2.4845053308  | 2.7837355614  |
| H43 | 3.2331064307  | 2.0988337765  | 2.9808744985  |
| H44 | 2.4801526763  | 3.3417367902  | 3.9878845561  |
| C45 | 4.2366850672  | 4.5999995140  | 2.2981565590  |
| H46 | 4.2390286636  | 4.9340909482  | 3.3416388075  |
| H47 | 5.0395401267  | 3.8609461244  | 2.1876770298  |
| H48 | 4.4830374397  | 5.4660062920  | 1.6788717848  |
| C49 | 4.9103208236  | -2.3877353108 | -1.1119581933 |
| H50 | 4.3835868373  | -1.9248997066 | -1.9512373811 |
| H51 | 5.6003347777  | -1.6513796104 | -0.6911441642 |
| H52 | 5.4994474151  | -3.2250621541 | -1.5030457683 |

|     |              |               |               |
|-----|--------------|---------------|---------------|
| C53 | 3.0671304695 | -4.0276870016 | -0.6876962996 |
| H54 | 2.5053164104 | -3.6524167870 | -1.5453442575 |
| H55 | 3.7344849475 | -4.8230563231 | -1.0398098766 |
| H56 | 2.3621074282 | -4.4772984721 | 0.0114903576  |
| C57 | 4.7459565920 | -3.4953983922 | 1.1257219811  |
| H58 | 5.4817146681 | -4.2033820837 | 0.7286110395  |
| H59 | 5.3020673992 | -2.7242908218 | 1.6721562148  |
| H60 | 4.1217876575 | -4.0414232837 | 1.8363553096  |
| C61 | 1.1075867737 | -3.1358722818 | 1.9523914632  |
| H62 | 0.5294128117 | -3.1686610142 | 1.0245489426  |
| H63 | 1.7528150112 | -4.0164895469 | 1.9929750842  |
| H64 | 0.4033481810 | -3.2100466276 | 2.7893104237  |
| C65 | 0.9051729046 | -0.6547992968 | 2.2512415926  |
| H66 | 0.1434518289 | -0.6284954931 | 1.4682398226  |
| H67 | 0.3854420616 | -0.7782958304 | 3.2080033336  |
| H68 | 1.4135084017 | 0.3134525103  | 2.2709441647  |
| C69 | 2.8127473167 | -1.8500246009 | 3.3188717404  |
| H70 | 2.1826781188 | -1.9429089218 | 4.2108748754  |
| H71 | 3.5064089337 | -2.6909056624 | 3.3268499395  |
| H72 | 3.3912066751 | -0.9268561875 | 3.4294791245  |
| N84 | 4.7106932175 | 0.7872617284  | -1.4402421531 |
| C85 | 5.4801412731 | 0.7843208306  | -2.3076334986 |
| C86 | 6.4515981633 | 0.7805948548  | -3.3932620670 |
| H87 | 6.4456967782 | 1.7476563597  | -3.9053085428 |
| H88 | 7.4537677192 | 0.5963958174  | -2.9940917424 |
| H89 | 6.2063892001 | -0.0058526813 | -4.1133315391 |
| C83 | 5.6109405203 | 0.6916625273  | 2.5343802023  |
| O84 | 5.5558468376 | 0.9536760074  | 1.3895659883  |
| O85 | 5.6265213628 | 0.4292135032  | 3.6678939541  |

**(P<sup>0</sup>N<sup>0</sup>P)Co<sup>0</sup>(NCCH<sub>3</sub>)<sub>2</sub> (N bound)**

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | -0.0018250096 | -0.4382372715 | 0.5487240934  |
| P2  | 2.3032348308  | 0.0333753147  | 0.2030743529  |
| P3  | -2.2989991263 | -0.0096981325 | 0.1160593067  |
| O4  | 2.3249430728  | 1.6990902392  | 0.0054678222  |
| C5  | 1.1369316575  | 2.3689139480  | -0.1573665454 |
| C6  | 1.1882238296  | 3.7066829177  | -0.4844775999 |
| H7  | 2.1586369294  | 4.1796865096  | -0.5879804521 |
| C8  | -0.0189767426 | 4.4048970847  | -0.6829653851 |
| H9  | -0.0230423801 | 5.4574047750  | -0.9420075445 |
| C10 | -1.2200571661 | 3.6800901826  | -0.5548642191 |
| H11 | -2.1930309266 | 4.1316758078  | -0.7150347428 |
| C12 | -1.1583897552 | 2.3437418589  | -0.2237010570 |
| N13 | -0.0086023118 | 1.6336396408  | 0.0049171095  |
| O14 | -2.3394589472 | 1.6492619057  | -0.1287662198 |
| C15 | 3.5434165138  | -0.0693976828 | 1.6365356612  |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| C16 | 3.0037968751  | 0.9106888605  | 2.7046285086  |
| H17 | 1.9401527058  | 0.7546923489  | 2.8992312933  |
| H18 | 3.1346164835  | 1.9480488833  | 2.3857650423  |
| H19 | 3.5553632678  | 0.7655432909  | 3.6429504271  |
| C20 | 4.9991667317  | 0.3141081942  | 1.3288276381  |
| H21 | 5.5753380736  | 0.3459904746  | 2.2634421301  |
| H22 | 5.0629517326  | 1.3020581440  | 0.8642767232  |
| H23 | 5.4880878658  | -0.4116723064 | 0.6730640799  |
| C24 | 3.4818270028  | -1.5094513600 | 2.1864845258  |
| H25 | 3.8703829151  | -2.2396824507 | 1.4691722760  |
| H26 | 2.4564062475  | -1.7959347679 | 2.4368419158  |
| H27 | 4.0935808168  | -1.5851439719 | 3.0951560870  |
| C28 | 3.1541758320  | -0.4275340594 | -1.4389147411 |
| C29 | 4.3155285940  | 0.4919345022  | -1.8634106318 |
| H30 | 5.2225802404  | 0.3279776599  | -1.2810627732 |
| H31 | 4.0341282779  | 1.5444200491  | -1.7736784160 |
| H32 | 4.5655164738  | 0.2977992437  | -2.9151021377 |
| C33 | 3.6121549243  | -1.8956380534 | -1.3929291510 |
| H34 | 3.9156446732  | -2.2232824685 | -2.3960848461 |
| H35 | 2.8093101070  | -2.5579343616 | -1.0507873562 |
| H36 | 4.4728094020  | -2.0348895936 | -0.7311631100 |
| C37 | 2.0299482588  | -0.2722205426 | -2.4902376724 |
| H38 | 2.4121824174  | -0.5511796836 | -3.4813239060 |
| H39 | 1.6800039902  | 0.7637379457  | -2.5450778121 |
| H40 | 1.1678086053  | -0.8989439187 | -2.2563957634 |
| C41 | -3.5745473730 | -0.0914223111 | 1.5205948023  |
| C42 | -3.0648686972 | 0.9162730595  | 2.5778805474  |
| H43 | -3.6374994282 | 0.7905488281  | 3.5063185251  |
| H44 | -3.1940134810 | 1.9452117599  | 2.2318723723  |
| H45 | -2.0052028758 | 0.7714715055  | 2.8006420849  |
| C46 | -3.5211488743 | -1.5178550245 | 2.1052811018  |
| H47 | -2.5008580581 | -1.7963635318 | 2.3834043098  |
| H48 | -3.8936418304 | -2.2657411348 | 1.3977985590  |
| H49 | -4.1514989306 | -1.5736391210 | 3.0026971612  |
| C50 | -5.0237980914 | 0.2785610605  | 1.1692208903  |
| H51 | -5.4954108683 | -0.4666833624 | 0.5226482365  |
| H52 | -5.0795432428 | 1.2532095203  | 0.6763773890  |
| H53 | -5.6213468035 | 0.3340304372  | 2.0892049408  |
| C54 | -3.1016435983 | -0.5220084294 | -1.5342523867 |
| C55 | -3.5360854441 | -1.9962130619 | -1.4635312802 |
| H56 | -3.8100275958 | -2.3530896818 | -2.4652144695 |
| H57 | -4.4100646761 | -2.1337155811 | -0.8191151971 |
| H58 | -2.7308607864 | -2.6363324836 | -1.0864178648 |
| C59 | -4.2678339160 | 0.3666540894  | -2.0087043051 |
| H60 | -4.0067623365 | 1.4258526937  | -1.9379052369 |
| H61 | -5.1858718672 | 0.2004141672  | -1.4445515674 |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| H62 | -4.4886464013 | 0.1429531361  | -3.0610754703 |
| C63 | -1.9553499271 | -0.3711234791 | -2.5618658170 |
| H64 | -1.0906496720 | -0.9812754060 | -2.2963953211 |
| H65 | -1.6188756828 | 0.6685603389  | -2.6285448719 |
| H66 | -2.3102663991 | -0.6745258351 | -3.5558842142 |
| N67 | 0.0340757505  | -2.2898768296 | -0.3428185378 |
| C69 | 0.0579062338  | -3.2367242067 | -1.0239004043 |
| C72 | 0.0899499449  | -4.3686547679 | -1.9414862624 |
| H73 | 0.0750655207  | -5.3196067143 | -1.3978688423 |
| H74 | -0.7782217603 | -4.3345830002 | -2.6083038574 |
| H75 | 0.9991502504  | -4.3301687416 | -2.5509908849 |
| N73 | -0.0323598972 | -0.8282515864 | 2.4725709036  |
| C75 | -0.0556265286 | -0.9306232858 | 3.6339033530  |
| C78 | -0.0917419112 | -0.9660154105 | 5.0899799629  |
| H79 | 0.6431663052  | -0.2647369293 | 5.5005872654  |
| H80 | -1.0856063646 | -0.6773033361 | 5.4486575870  |
| H81 | 0.1370037386  | -1.9689551342 | 5.4646763949  |

**(P<sup>O</sup>N<sup>O</sup>P)Co<sup>II</sup>( $\eta^2$ -NCCH<sub>3</sub>)<sub>2</sub> (C bound)**

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.6661147164  | 0.8218612191  | -0.1738968814 |
| N2  | 1.6457631718  | 1.0001656336  | 0.2179952357  |
| C3  | 1.0497092158  | 2.2107117969  | 0.2432159359  |
| C4  | -0.3119234250 | 2.3815632349  | 0.4940572687  |
| C5  | -1.0840843083 | 1.2373304340  | 0.6859146962  |
| C6  | -0.5028620384 | -0.0261477870 | 0.6005980937  |
| C7  | 0.8675639448  | -0.0943659931 | 0.3470459606  |
| H8  | -0.7276017434 | 3.3810782149  | 0.5168230857  |
| H9  | -2.1485015450 | 1.3302285368  | 0.8808848111  |
| H10 | -1.0700262150 | -0.9419836140 | 0.7099200992  |
| O11 | 1.8082297204  | 3.2917400962  | -0.0100836283 |
| O14 | 1.4437693624  | -1.3006998940 | 0.2035623598  |
| P17 | 3.4311272627  | 3.0464238104  | -0.5591168225 |
| P18 | 3.1212001076  | -1.3758941876 | -0.2113743602 |
| C19 | 3.6311945247  | -2.4938285352 | 1.2201804946  |
| C20 | 2.8978645559  | -2.3457155306 | -1.8263139701 |
| C21 | 4.2217210447  | 4.3230502385  | 0.5786951091  |
| C22 | 3.1642040588  | 3.7128040016  | -2.3162244670 |
| C25 | 2.5532360234  | 2.5093051402  | -3.0705552077 |
| H26 | 3.2112074599  | 1.6368561919  | -3.0265973168 |
| H27 | 1.5821471215  | 2.2209635779  | -2.6532752261 |
| H28 | 2.3986315541  | 2.7698263785  | -4.1250660351 |
| C29 | 2.1979126881  | 4.9047830114  | -2.4501686610 |
| H30 | 1.2476022635  | 4.7047178761  | -1.9489886113 |
| H31 | 2.6086953767  | 5.8293990986  | -2.0438506292 |
| H32 | 1.9894512308  | 5.0784925759  | -3.5138742677 |
| C33 | 4.5314085442  | 4.0513201693  | -2.9382536151 |



|     |                  |                    |                     |
|-----|------------------|--------------------|---------------------|
| H34 | 4.4127537811     | 4.2240967160       | -4.0152203532       |
| H35 | 4.9622315814     | 4.9587270398       | -2.5050197197       |
| H36 | 5.2503042244     | 3.2336155066       | -2.8100647952       |
| C37 | 3.7308640988     | 5.7635659460       | 0.3606553647        |
| H38 | 4.0883749960     | 6.1832117606       | -0.5840928774       |
| H39 | 2.6392694764     | 5.8265913581       | 0.3826415717        |
| H40 | 4.1198654398     | 6.3987890744       | 1.1663324583        |
| C41 | 3.8561408219     | 3.8754521374       | 2.0147553258        |
| H42 | 2.7842423725     | 3.9873323695       | 2.2019060847        |
| H43 | 4.1437769556     | 2.8362997924       | 2.1949524922        |
| H44 | 4.3921181177     | 4.5140524622       | 2.7279708096        |
| C45 | 5.7528547460     | 4.2496487700       | 0.4071212227        |
| H46 | 6.2208961602     | 4.9654752165       | 1.0941659843        |
| H47 | 6.1280165783     | 3.2542896530       | 0.6516403306        |
| H48 | 6.0743445936     | 4.5104866762       | -0.6055954231       |
| C49 | 2.6060570691     | -1.2479793528      | -2.8744237853       |
| H50 | 1.6931161627     | -0.6916443958      | -2.6351328919       |
| H51 | 3.4319241047     | -0.5325280804      | -2.9352291201       |
| H52 | 2.4712325378     | -1.7023648480      | -3.8639197623       |
| C53 | 1.7363674398     | -3.3574059826      | -1.8472468307       |
| H54 | 0.7935966498     | -2.8867024216      | -1.5584388470       |
| H55 | 1.6220741973     | -3.7488130216      | -2.8664248250       |
| H56 | 1.9058412212     | -4.2088783104      | -1.1874560480       |
| C57 | 4.2234548187     | -3.0394013503      | -2.1902052402       |
| H58 | 4.1735913764     | -3.4047641047      | -3.2233757672       |
| H59 | 5.0752692257     | -2.3525366726      | -2.1229957953       |
| H60 | 4.4242075521     | -3.8999580334      | -1.5460002892       |
| C61 | 2.9197901291     | -3.8569633096      | 1.2416078133        |
| H62 | 1.8335166958     | -3.7460745351      | 1.1792864710        |
| H63 | 3.2534780140     | -4.5114178817      | 0.4311976966        |
| H64 | 3.1513689590     | -4.3655834135      | 2.1859212589        |
| C65 | 3.2564947157     | -1.7083348210      | 2.5008221296        |
| H66 | 2.1713572421     | -1.6147229346      | 2.6052368043        |
| H67 | 3.6310528255     | -2.2588469954      | 3.3726658160        |
| H68 | 3.7038924279     | -0.7110124988      | 2.5012368939        |
| C69 | 5.1606660392     | -2.6890097150      | 1.1874272846        |
| H70 | 5.4566236658     | -3.2987346063      | 2.0502546607        |
| H71 | 5.4984248997     | -3.2114368873      | 0.2879662978        |
| H72 | 5.6804111412     | -1.7319795089      | 1.2587332131        |
| C80 | Co1 1.9600712840 | P17 101.1400437508 | N2 -155.1847858831  |
| N81 | C80 1.2221905581 | Co1 83.2547277763  | P17 92.3547877342   |
| C82 | C80 1.4985709615 | Co1 138.4277089315 | N81 179.3922330127  |
| H83 | C82 1.0958533843 | C80 109.8047034059 | Co1 58.1925386632   |
| H84 | C82 1.0973681332 | C80 111.5088400049 | H83 121.3487174350  |
| H85 | C82 1.0961389198 | C80 109.6302726136 | H83 -117.5368457941 |

**(P<sup>0</sup>N<sup>0</sup>P)Co<sup>0</sup>(NCCH<sub>3</sub>)CO<sub>2</sub>**

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.4530736272  | 0.8296145276  | 0.2558046245  |
| N2  | 1.4263715378  | 0.8070135860  | -0.3717444474 |
| C3  | 0.7447309723  | 1.9501181625  | -0.5564122929 |
| C4  | -0.5517361800 | 1.9798733652  | -1.0734552663 |
| C5  | -1.1430513114 | 0.7613801264  | -1.4011864611 |
| C6  | -0.4603551825 | -0.4368478534 | -1.1943431011 |
| C7  | 0.8243603719  | -0.3602193962 | -0.6564467025 |
| H8  | -1.0574702291 | 2.9293906495  | -1.1958480974 |
| H9  | -2.1513665982 | 0.7438249976  | -1.8044923026 |
| H10 | -0.8964663463 | -1.4050786191 | -1.4055563764 |
| O11 | 1.3368170644  | 3.1114042990  | -0.2090300736 |
| O12 | 1.4872784289  | -1.5011623353 | -0.3676942450 |
| P17 | 2.9680071803  | 3.0815490379  | 0.3441021287  |
| P18 | 2.8839033296  | -1.3950187228 | 0.6391000935  |
| C19 | 2.0747947858  | -1.7791220959 | 2.3163135031  |
| C20 | 3.7540325143  | -2.9349413585 | -0.0255117752 |
| C21 | 2.6810262883  | 3.8936934968  | 2.0245332499  |
| C22 | 3.7003605608  | 4.2985524174  | -0.8969710348 |
| C25 | 3.2377253474  | 3.8155056178  | -2.2910418001 |
| H26 | 3.4369227635  | 2.7542937131  | -2.4476722057 |
| H27 | 2.1670340155  | 3.9888220504  | -2.4316594661 |
| H28 | 3.7763543772  | 4.3817587841  | -3.0606633183 |
| C29 | 3.2884006526  | 5.7709830270  | -0.7394028374 |
| H30 | 2.2012756183  | 5.8911692569  | -0.7538616954 |
| H31 | 3.6773784991  | 6.2134393288  | 0.1808584404  |
| H32 | 3.6988136898  | 6.3487652777  | -1.5774483649 |
| C33 | 5.2343615928  | 4.1592129582  | -0.7752491786 |
| H34 | 5.7149624840  | 4.7266134319  | -1.5822734867 |
| H35 | 5.6055891852  | 4.5569465671  | 0.1737436898  |
| H36 | 5.5552476014  | 3.1166629674  | -0.8366823694 |
| C37 | 1.6996230272  | 5.0832870198  | 2.0220690736  |
| H38 | 2.1181923219  | 5.9848848694  | 1.5756047841  |
| H39 | 0.7705520231  | 4.8367166797  | 1.5004809782  |
| H40 | 1.4449623900  | 5.3245733756  | 3.0617880809  |
| C41 | 2.0717758808  | 2.7783745203  | 2.9032419606  |
| H42 | 1.0913307321  | 2.4687908793  | 2.5248007302  |
| H43 | 2.7374525321  | 1.9145406713  | 2.9539999678  |
| H44 | 1.9236186259  | 3.1627133200  | 3.9199523044  |
| C45 | 4.0472969203  | 4.2980017481  | 2.6133988093  |
| H46 | 3.9019296499  | 4.6297930824  | 3.6490473602  |
| H47 | 4.7380222438  | 3.4493427664  | 2.6268121542  |
| H48 | 4.5022211071  | 5.1301398737  | 2.0672696367  |
| C49 | 4.5410822485  | -2.4537866739 | -1.2636555666 |
| H50 | 3.8831460805  | -2.0038263188 | -2.0132145574 |
| H51 | 5.2948282592  | -1.7150525136 | -0.9836507526 |

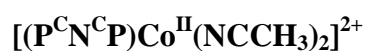
|     |              |               |               |
|-----|--------------|---------------|---------------|
| H52 | 5.0457306289 | -3.3125062050 | -1.7237656989 |
| C53 | 2.8133236466 | -4.0777898524 | -0.4576037402 |
| H54 | 2.0854694163 | -3.7363466946 | -1.1973563818 |
| H55 | 3.4154444068 | -4.8726444533 | -0.9153693770 |
| H56 | 2.2681343842 | -4.5210393217 | 0.3755810889  |
| C57 | 4.7663563485 | -3.4299241595 | 1.0269485971  |
| H58 | 5.4236487133 | -4.1760870573 | 0.5643857011  |
| H59 | 5.3998403309 | -2.6171816557 | 1.3992329559  |
| H60 | 4.2781447302 | -3.9081183023 | 1.8795510928  |
| C61 | 1.4190724605 | -3.1652446556 | 2.4344842035  |
| H62 | 0.6994347174 | -3.3420615375 | 1.6292661969  |
| H63 | 2.1503505341 | -3.9767903126 | 2.4368268153  |
| H64 | 0.8746096796 | -3.2192441180 | 3.3860706064  |
| C65 | 0.9676705846 | -0.7178740518 | 2.5102869886  |
| H66 | 0.1251012307 | -0.8759669311 | 1.8303232379  |
| H67 | 0.5835161935 | -0.7887064820 | 3.5347505443  |
| H68 | 1.3461005589 | 0.2924994864  | 2.3630343088  |
| C69 | 3.1380375418 | -1.5829506927 | 3.4201805770  |
| H70 | 2.6418059030 | -1.6227004149 | 4.3984167691  |
| H71 | 3.8946150695 | -2.3712694738 | 3.4090741275  |
| H72 | 3.6501922536 | -0.6217971071 | 3.3239308943  |
| N84 | 4.3628799264 | 0.7184744891  | -1.6509314575 |
| C85 | 5.4185975463 | 0.7203242078  | -2.1329209401 |
| C86 | 6.8108968535 | 0.7161223499  | -2.5470537487 |
| H87 | 7.0446932562 | 1.6006629032  | -3.1465168608 |
| H88 | 7.3907888386 | 0.7292106579  | -1.6167930251 |
| H89 | 7.0450106726 | -0.1842050933 | -3.1226462447 |
| C83 | 5.1965419597 | 0.8773368824  | 1.1385447063  |
| O84 | 4.7757324810 | 1.0171867232  | 2.3172842815  |
| O85 | 6.3184036229 | 0.7842370279  | 0.6253438004  |

**$[(P^ON^OP)Co^H(NCCH_3)H]^+$**

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 0.0380944199  | -0.3584249179 | -0.2300625211 |
| P2  | 2.2549866646  | 0.0055524272  | -0.0096860899 |
| P3  | -2.1969429590 | -0.0833609413 | -0.0671155521 |
| O4  | 2.3151407453  | 1.7025126375  | -0.2085901641 |
| C5  | 1.1545189649  | 2.3800443050  | -0.3014544677 |
| C6  | 1.1759884753  | 3.7714076917  | -0.3112479590 |
| H7  | 2.1250931947  | 4.2906627900  | -0.2763482171 |
| C8  | -0.0481979977 | 4.4378065241  | -0.3371843202 |
| H9  | -0.0691026032 | 5.5232209651  | -0.3388664006 |
| C10 | -1.2457038469 | 3.7245330200  | -0.3268051729 |
| H11 | -2.2145761946 | 4.2068059622  | -0.3058044922 |
| C12 | -1.1702979405 | 2.3348520146  | -0.3150599110 |
| N13 | 0.0055291986  | 1.6652335766  | -0.3554455118 |
| O14 | -2.3050922381 | 1.6145462378  | -0.2361351503 |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| C15 | 2.9501509852  | -0.1148424766 | 1.7302221995  |
| C16 | 1.8293528346  | 0.4496035098  | 2.6317254039  |
| H17 | 0.8963599371  | -0.1015165353 | 2.5056185945  |
| H18 | 1.6413148473  | 1.5098492283  | 2.4321456148  |
| H19 | 2.1317448287  | 0.3607120433  | 3.6808053090  |
| C20 | 4.2291961447  | 0.7069248972  | 1.9851623912  |
| H21 | 4.3969307228  | 0.7589913436  | 3.0669297776  |
| H22 | 4.1347637237  | 1.7308885931  | 1.6136335894  |
| H23 | 5.1169556962  | 0.2559245397  | 1.5440475777  |
| C24 | 3.1709234470  | -1.6044723256 | 2.0576666314  |
| H25 | 4.0055923673  | -2.0284536098 | 1.4917092503  |
| H26 | 2.2739277055  | -2.2010046277 | 1.8597317078  |
| H27 | 3.4138197934  | -1.7051058908 | 3.1213879730  |
| C28 | 3.4814645437  | -0.4566796872 | -1.3581594080 |
| C29 | 4.9326621970  | -0.0256994140 | -1.0746273414 |
| H30 | 5.3953291414  | -0.6244199499 | -0.2874806272 |
| H31 | 5.0019144154  | 1.0311115651  | -0.8037363185 |
| H32 | 5.5238788291  | -0.1736932843 | -1.9857922542 |
| C33 | 3.4210056168  | -1.9857747533 | -1.5574477680 |
| H34 | 4.0349069188  | -2.2550321856 | -2.4246651149 |
| H35 | 2.4029834164  | -2.3393252515 | -1.7308711368 |
| H36 | 3.8216870857  | -2.5253202054 | -0.6949647654 |
| C37 | 3.0114399638  | 0.2816495771  | -2.6362306203 |
| H38 | 3.5854337724  | -0.0966956934 | -3.4894882568 |
| H39 | 3.1972802288  | 1.3556902384  | -2.5578643896 |
| H40 | 1.9522636922  | 0.1343136595  | -2.8480738067 |
| C41 | -2.9765749255 | -0.2742588439 | 1.6340850544  |
| C42 | -1.8299732837 | 0.0072667965  | 2.6290188740  |
| H43 | -2.2126723930 | -0.0551830637 | 3.6535384579  |
| H44 | -1.4067694655 | 1.0093907155  | 2.4969660243  |
| H45 | -1.0299909061 | -0.7293534589 | 2.5202535863  |
| C46 | -3.4450700118 | -1.7315459929 | 1.8163179313  |
| H47 | -2.6565295287 | -2.4504914668 | 1.5677691099  |
| H48 | -4.3295857917 | -1.9599083590 | 1.2167028324  |
| H49 | -3.7136470089 | -1.8880420787 | 2.8670577073  |
| C50 | -4.1231826630 | 0.7176579222  | 1.9184001559  |
| H51 | -5.0111910224 | 0.5303705811  | 1.3159262038  |
| H52 | -3.8100746546 | 1.7521576424  | 1.7570389812  |
| H53 | -4.4141289731 | 0.6155735016  | 2.9700989845  |
| C54 | -3.3651632208 | -0.5601854023 | -1.4607630865 |
| C55 | -3.2547931246 | -2.0839999420 | -1.6822802991 |
| H56 | -3.8337310892 | -2.3547587859 | -2.5727133030 |
| H57 | -3.6620942075 | -2.6534354678 | -0.8433184136 |
| H58 | -2.2210401136 | -2.4013525492 | -1.8339417096 |
| C59 | -4.8327729940 | -0.1655423360 | -1.2100919521 |
| H60 | -4.9335232618 | 0.9000996517  | -0.9868527085 |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| H61 | -5.2904300538 | -0.7409780440 | -0.4027347883 |
| H62 | -5.4087275725 | -0.3685559821 | -2.1204361116 |
| C63 | -2.8789373314 | 0.2017251853  | -2.7178352286 |
| H64 | -1.8178807062 | 0.0520988734  | -2.9187777849 |
| H65 | -3.0626192935 | 1.2749906852  | -2.6241126930 |
| H66 | -3.4431449234 | -0.1594722730 | -3.5849003441 |
| N67 | 0.0831515558  | -1.2046382682 | -2.2165605910 |
| C68 | 0.1444064987  | -1.9078162008 | -3.1358849609 |
| C69 | 0.2301198672  | -2.8110970394 | -4.2756210925 |
| H70 | 0.7485496449  | -3.7284285575 | -3.9804728351 |
| H71 | -0.7742549568 | -3.0675234293 | -4.6253784518 |
| H72 | 0.7819227072  | -2.3357642682 | -5.0917045706 |
| H73 | 0.0598411197  | -1.7653794578 | 0.2970475570  |



|     |                  |                  |                   |
|-----|------------------|------------------|-------------------|
| Co1 | 3.4062705629     | 0.8856266940     | 0.4383675055      |
| N2  | 1.4167613839     | 1.1046014460     | 0.1824339728      |
| C3  | 0.8322892180     | 2.3007668453     | 0.4769934983      |
| C4  | -0.5461083557    | 2.4780065212     | 0.3979463312      |
| C5  | -1.3540503338    | 1.4155678990     | -0.0010278000     |
| C6  | -0.7507612597    | 0.2109907923     | -0.3480520680     |
| C7  | 0.6346743898     | 0.0860200074     | -0.2658660832     |
| H8  | -0.9740953093    | 3.4445814387     | 0.6410589833      |
| H9  | -2.4317031593    | 1.5328906074     | -0.0637493533     |
| H10 | -1.3405960848    | -0.6272324706    | -0.7028646211     |
| C11 | 1.7463141231     | 3.4318818289     | 0.8494381647      |
| H12 | 1.2839167593     | 4.3990055205     | 0.6410738702      |
| H13 | 1.9590403260     | 3.3915405808     | 1.9205101022      |
| C14 | 1.3271997318     | -1.1501525380    | -0.7588136165     |
| H15 | 0.6843957642     | -2.0309484283    | -0.6860293473     |
| H16 | 1.5449311955     | -1.0092996973    | -1.8240511606     |
| P17 | 3.3668528293     | 3.1797639776     | -0.0124555789     |
| P18 | 2.9470141752     | -1.3819690406    | 0.1004952486      |
| C19 | 2.5480840923     | -2.4425071874    | 1.6111328667      |
| C20 | 4.0021329601     | -2.2629629196    | -1.2024493904     |
| C21 | 4.5295982510     | 4.4476305841     | 0.7781749862      |
| C22 | 3.0184255382     | 3.5461883320     | -1.8615591061     |
| N24 | Co1 2.2118895118 | N2 89.6912429587 | P17 95.5491033332 |
| C25 | 2.4468376384     | 2.2713816487     | -2.5277587445     |
| H26 | 3.0934780988     | 1.4019033749     | -2.3714289963     |
| H27 | 1.4415781301     | 2.0280665464     | -2.1802801009     |
| H28 | 2.3824081059     | 2.4407517710     | -3.6080877952     |
| C29 | 1.9952010670     | 4.6867139882     | -2.0457276303     |
| H30 | 1.0091602498     | 4.4202223547     | -1.6532459951     |
| H31 | 2.3092446086     | 5.6261570948     | -1.5885112221     |
| H32 | 1.8695448083     | 4.8723752912     | -3.1182044558     |

|     |                  |                    |                    |
|-----|------------------|--------------------|--------------------|
| C33 | 4.3337742888     | 3.8952935254       | -2.5887504867      |
| H34 | 4.1272164777     | 3.9826086124       | -3.6608466861      |
| H35 | 4.7536786824     | 4.8493874162       | -2.2667597756      |
| H36 | 5.0933561043     | 3.1153796494       | -2.4677483199      |
| C37 | 4.1071488424     | 5.8960867281       | 0.4580142728       |
| H38 | 4.2279685684     | 6.1442584590       | -0.5981384959      |
| H39 | 3.0718657466     | 6.1028115454       | 0.7468957571       |
| H40 | 4.7434584973     | 6.5833395121       | 1.0264616560       |
| C41 | 4.4817981272     | 4.2353857006       | 2.3091375477       |
| H42 | 3.5200293857     | 4.5215752107       | 2.7442770242       |
| H43 | 4.7037902325     | 3.2015948115       | 2.5858974530       |
| H44 | 5.2397353987     | 4.8773472733       | 2.7697751337       |
| C45 | 5.9842898736     | 4.2011013455       | 0.3204178974       |
| H46 | 6.6363903685     | 4.9182623797       | 0.8306216950       |
| H47 | 6.3208737540     | 3.1974564659       | 0.5917637840       |
| H48 | 6.1303903338     | 4.3373107402       | -0.7502829371      |
| C49 | 4.3896733780     | -1.1941181138      | -2.2513701002      |
| H50 | 3.5188320110     | -0.8012440224      | -2.7856695162      |
| H51 | 4.9328472543     | -0.3530903974      | -1.8118279322      |
| H52 | 5.0381441749     | -1.6534181694      | -3.0050195003      |
| C53 | 3.2442035361     | -3.3975766620      | -1.9277345007      |
| H54 | 2.3426255853     | -3.0451985009      | -2.4367316644      |
| H55 | 3.9009836253     | -3.8130241975      | -2.6999421388      |
| H56 | 2.9661966772     | -4.2158967552      | -1.2646259928      |
| C57 | 5.2809369109     | -2.8302366886      | -0.5548336655      |
| H58 | 5.9425163342     | -3.2066265519      | -1.3423692937      |
| H59 | 5.8312176898     | -2.0720094202      | 0.0093590038       |
| H60 | 5.0677002395     | -3.6670707784      | 0.1138060983       |
| C61 | 2.2279585631     | -3.9100324354      | 1.2677559980       |
| H62 | 1.4200331106     | -4.0036668192      | 0.5353355892       |
| H63 | 3.0990191956     | -4.4539780420      | 0.8974009047       |
| H64 | 1.8940416782     | -4.4162762053      | 2.1803093355       |
| C65 | 1.3035744097     | -1.8177101562      | 2.2864835214       |
| H66 | 0.3922577262     | -1.9800338836      | 1.7038651296       |
| H67 | 1.1523825535     | -2.3037510153      | 3.2562749216       |
| H68 | 1.4137199273     | -0.7460718203      | 2.4605157955       |
| C69 | 3.7469553469     | -2.3733352513      | 2.5808486013       |
| H70 | 3.4989584458     | -2.9248196920      | 3.4941740999       |
| H71 | 4.6463971987     | -2.8297451970      | 2.1614298243       |
| H72 | 3.9811329575     | -1.3427437527      | 2.8588733104       |
| N73 | 5.3125035963     | 0.6681143616       | 0.5391449226       |
| C74 | N73 1.1564081622 | Co1 178.3015616586 | N24 151.2042588979 |
| C75 | N24 1.1590978887 | Co1 173.4320212624 | N2 -11.5472860757  |
| C76 | C75 1.4572814646 | N24 179.6005786276 | N2 34.8730751850   |
| H77 | C76 1.0946419753 | C75 109.8086322840 | N2 13.5695062272   |
| H78 | C76 1.0942312058 | C75 109.9366168571 | H77 119.8844378723 |

|     |     |              |     |                |     |                 |
|-----|-----|--------------|-----|----------------|-----|-----------------|
| H79 | C76 | 1.0945048180 | C75 | 110.0200778697 | H77 | -120.0533309222 |
| C80 | C74 | 1.4548087223 | N73 | 179.4188984197 | N2  | 31.8104887749   |
| H81 | C80 | 1.0946826002 | C74 | 109.9113176235 | N2  | 130.6290112540  |
| H82 | C80 | 1.0945216784 | C74 | 109.9794832356 | H81 | 120.2562313909  |
| H83 | C80 | 1.0948819813 | C74 | 109.5134792840 | H81 | -119.7988962313 |



|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.3426199985  | 0.8526370226  | 0.2568665025  |
| N2  | 1.5933197485  | 0.8044611969  | -0.6953024643 |
| C3  | 0.7942137507  | 1.9040753542  | -0.7807519592 |
| C4  | -0.3316944864 | 1.9207541825  | -1.5992949386 |
| C5  | -0.6717570583 | 0.7825524672  | -2.3242495796 |
| C6  | 0.1076965245  | -0.3616549376 | -2.1782546466 |
| C7  | 1.2254019491  | -0.3324891442 | -1.3486489279 |
| H8  | -0.9410006758 | 2.8166769413  | -1.6472114759 |
| H9  | -1.5460635050 | 0.7775944985  | -2.9678346104 |
| H10 | -0.1520899254 | -1.2833946889 | -2.6876437555 |
| C11 | 1.1222066020  | 3.0628148053  | 0.1139076354  |
| H12 | 0.7218818470  | 4.0019113770  | -0.2752106341 |
| H13 | 0.6294679446  | 2.8912350081  | 1.0783368892  |
| C14 | 2.0330466012  | -1.5771873724 | -1.0995441971 |
| H15 | 1.3955340015  | -2.4642677219 | -1.1510421862 |
| H16 | 2.8013775084  | -1.6872334803 | -1.8731257589 |
| P17 | 2.9409762015  | 3.1469083116  | 0.4328293073  |
| P18 | 2.9416343000  | -1.4334416064 | 0.5040104260  |
| C19 | 1.6926726318  | -1.7562977779 | 1.9037173015  |
| C20 | 4.2783341314  | -2.7741409647 | 0.3898428836  |
| C21 | 3.0521872122  | 3.8265154086  | 2.1956066566  |
| C22 | 3.6186605351  | 4.2998438146  | -0.8947886119 |
| C25 | 3.0336006700  | 3.8153475060  | -2.2435998479 |
| H26 | 3.1877849163  | 2.7467723560  | -2.4087465569 |
| H27 | 1.9637836815  | 4.0252043316  | -2.3307255306 |
| H28 | 3.5310173343  | 4.3579256560  | -3.0544263828 |
| C29 | 3.2174632227  | 5.7719259759  | -0.6819927149 |
| H30 | 2.1349095441  | 5.9058530984  | -0.5915835175 |
| H31 | 3.6976046861  | 6.2123742326  | 0.1941523699  |
| H32 | 3.5407494720  | 6.3510714564  | -1.5539505527 |
| C33 | 5.1563732993  | 4.1693123083  | -0.9238944520 |
| H34 | 5.5475051360  | 4.7683786357  | -1.7531668459 |
| H35 | 5.6233942153  | 4.5404917986  | -0.0095361616 |
| H36 | 5.4728927146  | 3.1344789490  | -1.0745167544 |
| C37 | 2.0801359820  | 4.9991685141  | 2.4504032978  |
| H38 | 2.2927569131  | 5.8690811689  | 1.8297049368  |
| H39 | 1.0329498424  | 4.7191540795  | 2.3044464795  |
| H40 | 2.1817095438  | 5.3119557168  | 3.4954679583  |
| C41 | 2.6666804634  | 2.6567060959  | 3.1302937031  |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| H42 | 1.6620958591  | 2.2655758381  | 2.9355623370  |
| H43 | 3.3751167445  | 1.8267484546  | 3.0573812034  |
| H44 | 2.6765896278  | 3.0037994177  | 4.1687435185  |
| C45 | 4.4966310273  | 4.2667810700  | 2.5062104170  |
| H46 | 4.5791574393  | 4.4945308431  | 3.5743110698  |
| H47 | 5.2293291245  | 3.4868993835  | 2.2746205733  |
| H48 | 4.7760368974  | 5.1713781248  | 1.9616754449  |
| C49 | 5.4006411269  | -2.2187493401 | -0.5146764603 |
| H50 | 5.0516619499  | -2.0134693947 | -1.5304916614 |
| H51 | 5.8392733771  | -1.2995999880 | -0.1162099077 |
| H52 | 6.1952071495  | -2.9682940904 | -0.5888687325 |
| C53 | 3.7305406275  | -4.0745087870 | -0.2417143382 |
| H54 | 3.3864962060  | -3.9295517007 | -1.2694731830 |
| H55 | 4.5428239244  | -4.8084056527 | -0.2785516974 |
| H56 | 2.9186404930  | -4.5197357844 | 0.3337803179  |
| C57 | 4.8741499816  | -3.0916729454 | 1.7766343520  |
| H58 | 5.7217203390  | -3.7721492411 | 1.6456684573  |
| H59 | 5.2545476188  | -2.2058738849 | 2.2938460776  |
| H60 | 4.1613307358  | -3.5919246922 | 2.4341875759  |
| C61 | 1.2270059640  | -3.2240760022 | 1.9652734654  |
| H62 | 0.7769718641  | -3.5565774648 | 1.0245145593  |
| H63 | 2.0316070811  | -3.9118504138 | 2.2296575278  |
| H64 | 0.4577153540  | -3.3161339441 | 2.7400776927  |
| C65 | 0.4491233136  | -0.8604114479 | 1.6956913943  |
| H66 | -0.1044572779 | -1.1047908570 | 0.7850174723  |
| H67 | -0.2314531963 | -1.0171712234 | 2.5392157476  |
| H68 | 0.7037590765  | 0.2029978032  | 1.6728029973  |
| C69 | 2.3489220014  | -1.3397780230 | 3.2396945446  |
| H70 | 1.6147466654  | -1.4471051798 | 4.0453769923  |
| H71 | 3.2115347273  | -1.9503706459 | 3.5070674335  |
| H72 | 2.6557521973  | -0.2882880200 | 3.2242014423  |
| N84 | 4.5103493464  | 0.7384595021  | -1.5293517296 |
| C85 | 5.1090003698  | 0.7018292199  | -2.5204704795 |
| C86 | 5.8610933330  | 0.6679463155  | -3.7671226009 |
| H87 | 5.7476531222  | 1.6206466156  | -4.2937499488 |
| H88 | 6.9216383240  | 0.4995064921  | -3.5567423204 |
| H89 | 5.4910329886  | -0.1395740877 | -4.4063069518 |
| C83 | 5.7004423995  | 0.4723367063  | 2.2939254559  |
| O84 | 5.1119682656  | 0.9265644860  | 1.3782969629  |
| O85 | 6.2886985998  | 0.0352292725  | 3.1874823034  |

**$[(P^C N^C P)Co^I(NCCH_3)_2]^+$**

|     |               |              |               |
|-----|---------------|--------------|---------------|
| Co1 | 3.9925862650  | 0.8180867846 | 0.2641656943  |
| N2  | 1.7821408811  | 0.7838722476 | -0.6315320593 |
| C3  | 1.0651909397  | 1.9168364881 | -0.7304640359 |
| C4  | -0.0640472873 | 1.9965267444 | -1.5469410645 |



|     |               |               |               |
|-----|---------------|---------------|---------------|
| C5  | -0.4714988367 | 0.8565963572  | -2.2393408094 |
| C6  | 0.2395262531  | -0.3309121795 | -2.0763346248 |
| C7  | 1.3683046852  | -0.3323525150 | -1.2517557179 |
| H8  | -0.6219112926 | 2.9249335618  | -1.6176592826 |
| H9  | -1.3487997268 | 0.8877842122  | -2.8791031937 |
| H10 | -0.0759672140 | -1.2448693538 | -2.5701560475 |
| C11 | 1.4883250257  | 3.0534124205  | 0.1708395432  |
| H12 | 1.0875516895  | 4.0102411690  | -0.1751065656 |
| H13 | 1.0391228248  | 2.8676264977  | 1.1538005858  |
| C14 | 2.1555032578  | -1.6011314708 | -0.9935469707 |
| H15 | 1.4703350424  | -2.4502321176 | -0.8976008185 |
| H16 | 2.7891481518  | -1.8133349453 | -1.8626265123 |
| P17 | 3.3345577966  | 3.1045404795  | 0.4408536182  |
| P18 | 3.3157210637  | -1.4511708266 | 0.4614150765  |
| C19 | 2.2236331007  | -1.8101952131 | 1.9830404425  |
| C20 | 4.5111577168  | -2.8963574631 | 0.1316430342  |
| C21 | 3.4511165770  | 3.8670565159  | 2.1763143959  |
| C22 | 3.9093052656  | 4.3172028223  | -0.9061905385 |
| C25 | 3.2657283327  | 3.8377062927  | -2.2300868506 |
| H26 | 3.3998014267  | 2.7659509203  | -2.3898169034 |
| H27 | 2.1938715491  | 4.0522127322  | -2.2705066426 |
| H28 | 3.7327081340  | 4.3701026777  | -3.0675356143 |
| C29 | 3.5188161115  | 5.7883222767  | -0.6834728680 |
| H30 | 2.4412104256  | 5.9150843403  | -0.5369382001 |
| H31 | 4.0363666927  | 6.2295561974  | 0.1716036981  |
| H32 | 3.7959420908  | 6.3744830660  | -1.5684977970 |
| C33 | 5.4434141031  | 4.1946914457  | -1.0299383997 |
| H34 | 5.7920504977  | 4.8023134419  | -1.8741769287 |
| H35 | 5.9597645685  | 4.5519837292  | -0.1355816370 |
| H36 | 5.7462219683  | 3.1586253352  | -1.2020251125 |
| C37 | 2.4835623003  | 5.0314159354  | 2.4661943381  |
| H38 | 2.6719002747  | 5.9026957707  | 1.8383966842  |
| H39 | 1.4359308056  | 4.7423914867  | 2.3399172497  |
| H40 | 2.6045181390  | 5.3476641013  | 3.5094171032  |
| C41 | 3.1289687500  | 2.7056789254  | 3.1474825027  |
| H42 | 2.1127366589  | 2.3178609575  | 3.0172939390  |
| H43 | 3.8260641823  | 1.8730099505  | 3.0186111322  |
| H44 | 3.2080649416  | 3.0602027250  | 4.1823060141  |
| C45 | 4.9028432899  | 4.3197350400  | 2.4300442600  |
| H46 | 5.0264164676  | 4.5708199892  | 3.4903937950  |
| H47 | 5.6201841485  | 3.5304954771  | 2.1830075223  |
| H48 | 5.1621693566  | 5.2120384299  | 1.8544059974  |
| C49 | 5.4980086737  | -2.3793918026 | -0.9402451774 |
| H50 | 4.9960535113  | -2.1407474360 | -1.8833841450 |
| H51 | 6.0200104484  | -1.4802669836 | -0.6034198107 |
| H52 | 6.2405792035  | -3.1576697161 | -1.1535222791 |

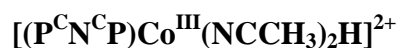
|     |                  |                    |                     |
|-----|------------------|--------------------|---------------------|
| C53 | 3.8526928156     | -4.1894896502      | -0.3906475047       |
| H54 | 3.3340281529     | -4.0345761012      | -1.3412618784       |
| H55 | 4.6310612248     | -4.9411153942      | -0.5700408235       |
| H56 | 3.1416604579     | -4.6195890279      | 0.3153863580        |
| C57 | 5.3209590403     | -3.2057071028      | 1.4066437873        |
| H58 | 6.1387257764     | -3.8927094838      | 1.1581587929        |
| H59 | 5.7653261112     | -2.2995020454      | 1.8320927814        |
| H60 | 4.7152999010     | -3.6904050126      | 2.1762605376        |
| C61 | 1.6956355702     | -3.2512012124      | 2.0871355874        |
| H62 | 1.1389657449     | -3.5524594584      | 1.1936241449        |
| H63 | 2.4952403989     | -3.9762329067      | 2.2542882553        |
| H64 | 1.0069656525     | -3.3265693531      | 2.9376751998        |
| C65 | 1.0119163182     | -0.8505326703      | 1.9345321652        |
| H66 | 0.3364899537     | -1.0689808079      | 1.1022311902        |
| H67 | 0.4364528804     | -0.9609510062      | 2.8611532293        |
| H68 | 1.3246463189     | 0.1934936568       | 1.8514547904        |
| C69 | 3.0402588728     | -1.4524381342      | 3.2455848692        |
| H70 | 2.3970328857     | -1.5307716576      | 4.1304516745        |
| H71 | 3.8923271463     | -2.1166821532      | 3.4012920854        |
| H72 | 3.4147481029     | -0.4251612555      | 3.1934190134        |
| N73 | 5.7271517856     | 0.7680087120       | 1.4619384537        |
| C74 | N73 1.1618133342 | Co1 165.9455348863 | N2 -1.0402262631    |
| C80 | C74 1.4581652319 | N73 179.4091428776 | N2 2.0666271672     |
| H81 | C80 1.0940167037 | C74 110.0800634882 | N2 167.2467972929   |
| H82 | C80 1.0943853347 | C74 110.0549509239 | H81 119.9472834375  |
| H83 | C80 1.0944202347 | C74 110.0701222009 | H81 -120.0049127386 |
| N84 | Co1 2.0504778340 | N2 90.6105999242   | H26 -43.5203053740  |
| C85 | N84 1.1610310739 | Co1 175.5387875375 | N2 13.2046899055    |
| C86 | C85 1.4582960771 | N84 178.8875190723 | N2 57.7153483298    |
| H87 | C86 1.0947163282 | C85 109.8988508012 | H26 14.5428653571   |
| H88 | C86 1.0941213077 | C85 110.2194154346 | H87 119.9652786505  |
| H89 | C86 1.0944200671 | C85 110.2640539659 | H87 -119.9044986111 |

$[(P^C N^C P)Co^I(NCCH_3)CO_2]^+$

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.3348428264  | 0.8990316211  | 1.0326147062  |
| N2  | 1.7440650112  | 1.1059464331  | -0.2320136050 |
| C3  | 1.0883150728  | 2.2935185090  | -0.3373520799 |
| C4  | -0.0242480231 | 2.4518340714  | -1.1599702894 |
| C5  | -0.4912963432 | 1.3707433466  | -1.9002539665 |
| C6  | 0.2012167502  | 0.1680323418  | -1.8253078689 |
| C7  | 1.3223589130  | 0.0707907867  | -1.0027501261 |
| H8  | -0.5178457931 | 3.4166065909  | -1.2049659105 |
| H9  | -1.3668511015 | 1.4691484165  | -2.5347911620 |
| H10 | -0.1060210470 | -0.6933933788 | -2.4084242404 |
| C11 | 1.6015454331  | 3.4412292540  | 0.4799548020  |
| H12 | 1.3957424471  | 4.4009573095  | -0.0006826751 |

|     |              |               |               |
|-----|--------------|---------------|---------------|
| H13 | 1.0754354669 | 3.4202529834  | 1.4373163448  |
| C14 | 2.1576948197 | -1.1752939991 | -1.0001387171 |
| H15 | 1.5631094775 | -2.0553220206 | -1.2581379695 |
| H16 | 2.9202460052 | -1.0696906962 | -1.7800906306 |
| P17 | 3.3819737931 | 3.1619685427  | 0.8752326242  |
| P18 | 3.0526435659 | -1.3587836096 | 0.6088417305  |
| C19 | 1.8666024475 | -2.4196478955 | 1.6518504692  |
| C20 | 4.6080680304 | -2.3136463721 | 0.0828990983  |
| C21 | 3.7460769511 | 4.3649036605  | 2.3045916698  |
| C22 | 4.3500149159 | 3.6191174923  | -0.7042468694 |
| C25 | 4.1783167647 | 2.4618195144  | -1.7206268267 |
| H26 | 4.4877061327 | 1.4974303454  | -1.3034396638 |
| H27 | 3.1492698830 | 2.3669089198  | -2.0746051860 |
| H28 | 4.8084313895 | 2.6662060595  | -2.5942456114 |
| C29 | 3.8695817573 | 4.9125100805  | -1.3916135436 |
| H30 | 2.8221062058 | 4.8406459723  | -1.7008770649 |
| H31 | 3.9843326385 | 5.8020730783  | -0.7738987163 |
| H32 | 4.4599494549 | 5.0681748902  | -2.3021741144 |
| C33 | 5.8500661887 | 3.7083038704  | -0.3541877915 |
| H34 | 6.4272992011 | 3.8348220258  | -1.2772488245 |
| H35 | 6.0841548605 | 4.5548022361  | 0.2941732482  |
| H36 | 6.2012567587 | 2.7915580055  | 0.1318484982  |
| C37 | 3.9579832651 | 5.8183029955  | 1.8364398863  |
| H38 | 4.8538444064 | 5.9463398256  | 1.2264820462  |
| H39 | 3.0970372857 | 6.1982821268  | 1.2773935090  |
| H40 | 4.0744104544 | 6.4551404071  | 2.7207464396  |
| C41 | 2.5565153313 | 4.3721725345  | 3.2954481670  |
| H42 | 1.6724945176 | 4.8622550352  | 2.8781166272  |
| H43 | 2.2764441592 | 3.3782865874  | 3.6447672594  |
| H44 | 2.8552360929 | 4.9516562100  | 4.1760363480  |
| C45 | 4.9892045320 | 3.8548754085  | 3.0654222323  |
| H46 | 5.2414854145 | 4.5729893746  | 3.8537231214  |
| H47 | 4.7778380935 | 2.8929641809  | 3.5378077384  |
| H48 | 5.8664634523 | 3.7513654180  | 2.4212935873  |
| C49 | 5.5136856302 | -1.3115569554 | -0.6733437196 |
| H50 | 5.0523469305 | -0.9558997007 | -1.6006805234 |
| H51 | 5.7690125705 | -0.4403832220 | -0.0697607174 |
| H52 | 6.4447597614 | -1.8162594324 | -0.9555129942 |
| C53 | 4.3330681031 | -3.4985365810 | -0.8688223181 |
| H54 | 3.8110098283 | -3.1912540697 | -1.7797931046 |
| H55 | 5.2932299374 | -3.9256602272 | -1.1807028421 |
| H56 | 3.7600964374 | -4.2977090169 | -0.4020676589 |
| C57 | 5.3424804871 | -2.8217621389 | 1.3391874598  |
| H58 | 6.3259569974 | -3.2119669373 | 1.0535686464  |
| H59 | 5.4933312008 | -2.0280537271 | 2.0760975073  |
| H60 | 4.7986302380 | -3.6354265744 | 1.8250423267  |

|     |               |               |              |
|-----|---------------|---------------|--------------|
| C61 | 1.7360774814  | -3.8744978817 | 1.1622875119 |
| H62 | 1.4756754811  | -3.9453966607 | 0.1013616720 |
| H63 | 2.6415977936  | -4.4588160004 | 1.3396712687 |
| H64 | 0.9265390730  | -4.3554699010 | 1.7234910197 |
| C65 | 0.4691790303  | -1.7591803954 | 1.5615250048 |
| H66 | 0.0265181553  | -1.8670212371 | 0.5663554426 |
| H67 | -0.1980992232 | -2.2716330666 | 2.2635448277 |
| H68 | 0.4775548957  | -0.7020298988 | 1.8264697540 |
| C69 | 2.3333768715  | -2.4191768437 | 3.1231388780 |
| H70 | 1.6054100314  | -2.9789125062 | 3.7213214362 |
| H71 | 3.3020592129  | -2.9087545087 | 3.2501619754 |
| H72 | 2.4058087496  | -1.4144468299 | 3.5401933404 |
| N73 | 5.0075424217  | 0.7276744524  | 1.9202861668 |
| C74 | 6.0142722040  | 0.6462056493  | 2.4827120097 |
| C80 | 7.2644913530  | 0.5566713788  | 3.2212542837 |
| H81 | 8.0980290884  | 0.3747628864  | 2.5359765999 |
| H82 | 7.4397280543  | 1.4936253119  | 3.7591433173 |
| H83 | 7.2094798549  | -0.2629041912 | 3.9443081987 |
| C83 | 2.2403423408  | 1.0650642416  | 2.8616229091 |
| O84 | 3.0101577415  | 0.8889599051  | 3.7785654332 |
| O85 | 1.0902806604  | 1.3216163072  | 2.5689939561 |



|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.5952874009  | 0.8074461092  | 0.6322989134  |
| N2  | 1.6652890399  | 0.8453205790  | -0.4152867106 |
| C3  | 1.0001351907  | 2.0108959315  | -0.5749414005 |
| C4  | -0.1059033773 | 2.1175127314  | -1.4175345645 |
| C5  | -0.5338992392 | 0.9925866511  | -2.1184632783 |
| C6  | 0.1725286465  | -0.1981811942 | -1.9751756187 |
| C7  | 1.2771243455  | -0.2370184994 | -1.1235267915 |
| H8  | -0.6166703316 | 3.0694491534  | -1.5194911540 |
| H9  | -1.3944556184 | 1.0481105985  | -2.7783117771 |
| H10 | -0.1128742359 | -1.0883198379 | -2.5262035875 |
| C11 | 1.5234860591  | 3.1903963172  | 0.1987100903  |
| H12 | 1.2414263781  | 4.1329095220  | -0.2791665454 |
| H13 | 1.0630408616  | 3.1924644133  | 1.1930561613  |
| C14 | 2.1274683554  | -1.4800838684 | -1.0230740262 |
| H15 | 1.5070063064  | -2.3810607748 | -0.9961367608 |
| H16 | 2.7341541458  | -1.5442951317 | -1.9338343198 |
| P17 | 3.3659981618  | 3.0556692416  | 0.4675633260  |
| P18 | 3.3199620792  | -1.3924056806 | 0.3891557296  |
| C19 | 2.3279600499  | -2.0860829806 | 1.8653062640  |
| C20 | 4.7101153694  | -2.5618821777 | -0.1466009646 |
| C21 | 3.5702350183  | 4.0747544030  | 2.0579218937  |
| C22 | 4.1358303981  | 3.8913887944  | -1.0468841326 |
| C25 | 3.4942310260  | 3.2282088882  | -2.2879011799 |

|     |              |               |               |
|-----|--------------|---------------|---------------|
| H26 | 3.5707605063 | 2.1384395081  | -2.2421920618 |
| H27 | 2.4417574088 | 3.5026958292  | -2.4083640306 |
| H28 | 4.0243203184 | 3.5704674400  | -3.1837561412 |
| C29 | 3.9132156767 | 5.4123348460  | -1.1222205722 |
| H30 | 2.8545582802 | 5.6854453143  | -1.0614591761 |
| H31 | 4.4549917231 | 5.9494927804  | -0.3401333418 |
| H32 | 4.2863180949 | 5.7796075847  | -2.0854282308 |
| C33 | 5.6465118819 | 3.5755638123  | -1.0557103688 |
| H34 | 6.0894009016 | 3.9682657179  | -1.9782484287 |
| H35 | 6.1745459087 | 4.0361692079  | -0.2172204919 |
| H36 | 5.8168152390 | 2.4958904893  | -1.0241615690 |
| C37 | 2.7798538708 | 5.4002616221  | 2.0742479005  |
| H38 | 3.1083466965 | 6.0995381452  | 1.3055553699  |
| H39 | 1.7032015308 | 5.2469451772  | 1.9574101738  |
| H40 | 2.9283733612 | 5.8881809856  | 3.0448510737  |
| C41 | 3.0411205502 | 3.1823190251  | 3.2078361208  |
| H42 | 1.9790649714 | 2.9380544342  | 3.0949046450  |
| H43 | 3.5970555715 | 2.2460155953  | 3.2896315096  |
| H44 | 3.1435344199 | 3.7206988203  | 4.1572836385  |
| C45 | 5.0641283160 | 4.3644072351  | 2.3013240330  |
| H46 | 5.1929870180 | 4.7863723027  | 3.3048515906  |
| H47 | 5.6706369293 | 3.4564190098  | 2.2358736532  |
| H48 | 5.4596480766 | 5.0935681776  | 1.5896636788  |
| C49 | 5.5813540037 | -1.7837485471 | -1.1592804826 |
| H50 | 5.0126533388 | -1.4577777049 | -2.0360060221 |
| H51 | 6.0232644391 | -0.8925721249 | -0.7087888896 |
| H52 | 6.3853415725 | -2.4403381230 | -1.5124086921 |
| C53 | 4.2039096499 | -3.8533540611 | -0.8245019401 |
| H54 | 3.6382765289 | -3.6476714502 | -1.7376912506 |
| H55 | 5.0685469792 | -4.4609969301 | -1.1152726577 |
| H56 | 3.5823694187 | -4.4643368527 | -0.1695475690 |
| C57 | 5.5858539477 | -2.9248404397 | 1.0697105719  |
| H58 | 6.4761297285 | -3.4617350348 | 0.7225879139  |
| H59 | 5.9227171492 | -2.0316784095 | 1.6052902964  |
| H60 | 5.0677641401 | -3.5790993595 | 1.7753531373  |
| C61 | 2.0064956213 | -3.5878370165 | 1.7743568707  |
| H62 | 1.4909029321 | -3.8481987267 | 0.8444367009  |
| H63 | 2.9002476949 | -4.2099448122 | 1.8588641370  |
| H64 | 1.3399059494 | -3.8634149045 | 2.6005806328  |
| C65 | 0.9946827127 | -1.3021212332 | 1.9261546651  |
| H66 | 0.3445286620 | -1.5066104142 | 1.0708502174  |
| H67 | 0.4497729065 | -1.6011307463 | 2.8286291438  |
| H68 | 1.1560665604 | -0.2209603817 | 1.9752881403  |
| C69 | 3.0940850535 | -1.7895209695 | 3.1732180812  |
| H70 | 2.4929039009 | -2.1255629184 | 4.0263734061  |
| H71 | 4.0562634089 | -2.3024647109 | 3.2269152705  |

|     |              |               |               |
|-----|--------------|---------------|---------------|
| H72 | 3.2751707656 | -0.7174455826 | 3.2933618416  |
| N73 | 5.0907856650 | 0.7234061769  | 2.0622134191  |
| C74 | 6.0623884846 | 0.6465552675  | 2.6914381368  |
| C80 | 7.2931011036 | 0.5484512158  | 3.4660700558  |
| H81 | 8.1457132389 | 0.4125512280  | 2.7934215354  |
| H82 | 7.4435318718 | 1.4618174598  | 4.0493340230  |
| H83 | 7.2397984447 | -0.3048792931 | 4.1488458183  |
| H77 | 4.3822755891 | 0.7721124660  | -0.6423928040 |

**(P<sup>C</sup>N<sup>C</sup>P)Co<sup>0</sup>(NCCH<sub>3</sub>)<sub>2</sub> (N-bound)**

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.9516136282  | 0.8131675961  | 0.1088085076  |
| N2  | 1.9169742091  | 0.7943547098  | -0.6312099457 |
| C3  | 1.1050319755  | 1.9182582076  | -0.6679767875 |
| C4  | -0.0733090441 | 1.9794845037  | -1.3798193173 |
| C5  | -0.5452456578 | 0.8471913143  | -2.0822463563 |
| C6  | 0.2077162611  | -0.3393074679 | -1.9407572032 |
| C7  | 1.3870248576  | -0.3422337411 | -1.2249706073 |
| H8  | -0.6532426385 | 2.9000772708  | -1.3581258453 |
| H9  | -1.4702951835 | 0.8716278241  | -2.6474543397 |
| H10 | -0.1394862689 | -1.2708559868 | -2.3838802227 |
| C11 | 1.5333814094  | 3.0388854900  | 0.2441831836  |
| H12 | 1.1037142044  | 3.9999358767  | -0.0573364525 |
| H13 | 1.1463009668  | 2.8186327628  | 1.2494777586  |
| C14 | 2.1763891766  | -1.6168895977 | -1.0200895054 |
| H15 | 1.5059137952  | -2.4807573692 | -0.9488752836 |
| H16 | 2.8386175665  | -1.7973164724 | -1.8789485069 |
| P17 | 3.3775533258  | 3.0992513918  | 0.4498812038  |
| P18 | 3.3292694214  | -1.4604055191 | 0.4264816553  |
| C19 | 2.2428975839  | -1.8387225570 | 1.9624169599  |
| C20 | 4.5258953519  | -2.9226855795 | 0.1227104875  |
| C21 | 3.5287386981  | 3.9043787459  | 2.1775162393  |
| C22 | 3.9210436430  | 4.3376813588  | -0.9020182138 |
| C25 | 3.2624738833  | 3.8323343489  | -2.2079857158 |
| H26 | 3.4133942601  | 2.7593617423  | -2.3448489409 |
| H27 | 2.1844394030  | 4.0131727202  | -2.2226819032 |
| H28 | 3.7019590463  | 4.3621385419  | -3.0640456868 |
| C29 | 3.5182468056  | 5.8061226119  | -0.6918873522 |
| H30 | 2.4426529106  | 5.9166485597  | -0.5192314844 |
| H31 | 4.0496244295  | 6.2655084862  | 0.1463374944  |
| H32 | 3.7653080688  | 6.3882309003  | -1.5904951805 |
| C33 | 5.4528149299  | 4.2348535700  | -1.0572999820 |
| H34 | 5.7786500444  | 4.8264203947  | -1.9239218539 |
| H35 | 5.9843018438  | 4.6174161336  | -0.1814575479 |
| H36 | 5.7605731548  | 3.1971706921  | -1.2108706636 |
| C37 | 2.5770011929  | 5.0837949555  | 2.4620984683  |
| H38 | 2.7779936423  | 5.9509687043  | 1.8323510180  |

|     |                  |                    |                     |
|-----|------------------|--------------------|---------------------|
| H39 | 1.5278369013     | 4.8043328610       | 2.3274941008        |
| H40 | 2.6941261191     | 5.4035320147       | 3.5065465568        |
| C41 | 3.2076289276     | 2.7794308564       | 3.1903125931        |
| H42 | 2.1770391648     | 2.4220538288       | 3.0988084954        |
| H43 | 3.8650789056     | 1.9194154139       | 3.0519920354        |
| H44 | 3.3334420032     | 3.1602969870       | 4.2133053012        |
| C45 | 4.9862637548     | 4.3497295950       | 2.4046969538        |
| H46 | 5.1304725950     | 4.6264202980       | 3.4576567272        |
| H47 | 5.6907844884     | 3.5466835595       | 2.1644734097        |
| H48 | 5.2471177565     | 5.2241576631       | 1.8017911449        |
| C49 | 5.5182172304     | -2.4140500609      | -0.9483383808       |
| H50 | 5.0177703878     | -2.1825739550      | -1.8939249397       |
| H51 | 6.0270894755     | -1.5051740425      | -0.6178994316       |
| H52 | 6.2692789521     | -3.1895335382      | -1.1512868703       |
| C53 | 3.8813257099     | -4.2243957082      | -0.3936628605       |
| H54 | 3.3463952367     | -4.0672383101      | -1.3349534113       |
| H55 | 4.6641505213     | -4.9707532393      | -0.5865451908       |
| H56 | 3.1821001424     | -4.6619363224      | 0.3201940845        |
| C57 | 5.3356021866     | -3.2170226799      | 1.4008601953        |
| H58 | 6.1549773473     | -3.9098463819      | 1.1673829057        |
| H59 | 5.7778866631     | -2.3027113223      | 1.8112881032        |
| H60 | 4.7281808012     | -3.6852962161      | 2.1797952794        |
| C61 | 1.7577834880     | -3.2921866726      | 2.0912864769        |
| H62 | 1.2133956489     | -3.6192619816      | 1.1990485668        |
| H63 | 2.5768443745     | -3.9936583599      | 2.2702925439        |
| H64 | 1.0677128216     | -3.3764422879      | 2.9419123651        |
| C65 | 1.0013987539     | -0.9196498771      | 1.8955411976        |
| H66 | 0.3418379689     | -1.1706379035      | 1.0604288288        |
| H67 | 0.4275047289     | -1.0285033147      | 2.8254065711        |
| H68 | 1.2909243925     | 0.1278349674       | 1.7807268881        |
| C69 | 3.0445181536     | -1.4319204878      | 3.2180369756        |
| H70 | 2.4040025936     | -1.5071818863      | 4.1065963620        |
| H71 | 3.9178028834     | -2.0665742075      | 3.3884449176        |
| H72 | 3.3878861636     | -0.3964520230      | 3.1313250099        |
| N73 | 5.5482038089     | 0.7447822435       | 1.4891375265        |
| C74 | N73 1.1659347801 | Co1 168.6837928081 | N2 1.6515817776     |
| C80 | C74 1.4585023980 | N73 176.6967787263 | N2 -7.8277695790    |
| H81 | C80 1.0951964050 | C74 111.0437580376 | N2 170.0667745245   |
| H82 | C80 1.0953244447 | C74 109.9565266367 | H81 120.1806621575  |
| H83 | C80 1.0954682140 | C74 110.0883238843 | H81 -120.2771184610 |
| N84 | Co1 1.9699398631 | N2 98.5207970486   | H26 -44.3255421085  |
| C85 | N84 1.1653244160 | Co1 168.8002491338 | N2 3.6623396001     |
| C86 | C85 1.4577265428 | N84 176.8969484764 | N2 12.3898437545    |
| H87 | C86 1.0952153968 | C85 109.9747399888 | H26 12.5680961786   |
| H88 | C86 1.0947328869 | C85 110.9143438356 | H87 120.1346980173  |
| H89 | C86 1.0950066914 | C85 110.3412165897 | H87 -119.5448121329 |

**(P<sup>C</sup>N<sup>C</sup>P)Co<sup>II</sup>(η<sup>2</sup>-NCCH<sub>3</sub>) (C-bound)**

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.6310484492  | 0.7588276657  | -0.0222295895 |
| N2  | 1.6058238026  | 0.9991283967  | 0.3310206290  |
| C3  | 1.1506838084  | 2.1994277517  | 0.7823342567  |
| C4  | -0.2030928341 | 2.4365331137  | 1.0108151630  |
| C5  | -1.1259417459 | 1.4213787654  | 0.7605476074  |
| C6  | -0.6627573360 | 0.2100670837  | 0.2503778704  |
| C7  | 0.7030890800  | 0.0344503206  | 0.0284587960  |
| H8  | -0.5216521175 | 3.4074862032  | 1.3768410269  |
| H9  | -2.1859996606 | 1.5797182451  | 0.9359810784  |
| H10 | -1.3509693371 | -0.5916339776 | 0.0007527641  |
| C11 | 2.2040152227  | 3.2485675484  | 0.9662423405  |
| H12 | 1.7699006183  | 4.2466560512  | 1.0827159555  |
| H13 | 2.7783693734  | 3.0060062543  | 1.8661074073  |
| C14 | 1.2256015620  | -1.2002035008 | -0.6654945324 |
| H15 | 0.6420927620  | -2.0842679669 | -0.3902511179 |
| H16 | 1.0710432029  | -1.0502058116 | -1.7411211996 |
| P17 | 3.4735383283  | 3.0815243028  | -0.4089537552 |
| P18 | 3.0674957726  | -1.4011792266 | -0.4235324021 |
| C19 | 3.1455793240  | -2.5727785881 | 1.0730178319  |
| C20 | 3.5590645315  | -2.2873237965 | -2.0378509412 |
| C21 | 4.7532226914  | 4.4054584211  | 0.0974559380  |
| C22 | 2.5333267584  | 3.6445813861  | -1.9874703481 |
| C25 | 1.7455820395  | 2.4192585000  | -2.5120214202 |
| H26 | 2.3847431751  | 1.5341194340  | -2.5827084144 |
| H27 | 0.8939739081  | 2.1705833620  | -1.8755535293 |
| H28 | 1.3547016217  | 2.6431423047  | -3.5130065543 |
| C29 | 1.5320359547  | 4.7958848743  | -1.7744118800 |
| H30 | 0.7565596018  | 4.5223469300  | -1.0521271340 |
| H31 | 2.0075724508  | 5.7167648412  | -1.4335465384 |
| H32 | 1.0253810688  | 5.0187741125  | -2.7229749160 |
| C33 | 3.5546726153  | 4.0253260476  | -3.0793917922 |
| H34 | 3.0277865376  | 4.1975297499  | -4.0267467536 |
| H35 | 4.1040176727  | 4.9393573164  | -2.8438209647 |
| H36 | 4.2803888217  | 3.2219098114  | -3.2474685725 |
| C37 | 4.3091345903  | 5.8666122386  | -0.0975678805 |
| H38 | 4.1764116843  | 6.1342096233  | -1.1486213923 |
| H39 | 3.3755640473  | 6.0832196313  | 0.4324404102  |
| H40 | 5.0774284355  | 6.5350005757  | 0.3129884125  |
| C41 | 5.0734481601  | 4.1976087656  | 1.5982180318  |
| H42 | 4.2674598926  | 4.5672931700  | 2.2400304361  |
| H43 | 5.2594738182  | 3.1486330937  | 1.8438597583  |
| H44 | 5.9720471243  | 4.7760285775  | 1.8476746738  |
| C45 | 6.0474640354  | 4.1330821803  | -0.6992687880 |
| H46 | 6.8269774123  | 4.8370547125  | -0.3812256423 |



|     |                  |                    |                     |
|-----|------------------|--------------------|---------------------|
| H47 | 6.4098243043     | 3.1190523797       | -0.5124327655       |
| H48 | 5.9162446368     | 4.2538974911       | -1.7770608293       |
| C49 | 3.6375885550     | -1.1585845093      | -3.0919431139       |
| H50 | 2.6576872495     | -0.7095407638      | -3.2886823376       |
| H51 | 4.3131343377     | -0.3607938779      | -2.7645099252       |
| H52 | 4.0067824676     | -1.5621374083      | -4.0434985137       |
| C53 | 2.5851436354     | -3.3704395971      | -2.5414112496       |
| H54 | 1.5782980502     | -2.9772541402      | -2.7121224096       |
| H55 | 2.9430953085     | -3.7637187480      | -3.5018774330       |
| H56 | 2.5046748714     | -4.2130559717      | -1.8527213533       |
| C57 | 4.9652425200     | -2.8970799099      | -1.8827057348       |
| H58 | 5.3361562621     | -3.2206731065      | -2.8635961191       |
| H59 | 5.6769661610     | -2.1696089323      | -1.4797121060       |
| H60 | 4.9611787195     | -3.7742070960      | -1.2297555147       |
| C61 | 2.5528335372     | -3.9722440939      | 0.8391615801        |
| H62 | 1.5323523538     | -3.9385154397      | 0.4426170694        |
| H63 | 3.1654659207     | -4.5665016600      | 0.1551489673        |
| H64 | 2.5122031029     | -4.5145390129      | 1.7928491916        |
| C65 | 2.3530353071     | -1.8530551167      | 2.1907127696        |
| H66 | 1.2792024831     | -1.8125906190      | 1.9805778353        |
| H67 | 2.4813512132     | -2.4035000864      | 3.1308254459        |
| H68 | 2.7221676525     | -0.8330067837      | 2.3339603762        |
| C69 | 4.6081390856     | -2.7000299212      | 1.5499286760        |
| H70 | 4.6342412681     | -3.3136651946      | 2.4598082928        |
| H71 | 5.2503954120     | -3.1858319177      | 0.8116981481        |
| H72 | 5.0250388513     | -1.7201893317      | 1.7900842815        |
| C80 | Co1 1.9480079365 | P17 101.3400971446 | N2 -149.6899862203  |
| N81 | C80 1.2280878884 | Co1 80.8169325967  | P17 88.6338555250   |
| C82 | C80 1.5008482477 | Co1 142.7102103647 | N81 175.6555200864  |
| H83 | C82 1.0947872158 | C80 110.8995093871 | Co1 47.6890365659   |
| H84 | C82 1.0974860594 | C80 111.6682159410 | H83 122.5349883197  |
| H85 | C82 1.0970369301 | C80 108.9424674398 | H83 -117.5862632796 |

**(P<sup>C</sup>N<sup>C</sup>P)Co<sup>0</sup>(NCCH<sub>3</sub>)CO<sub>2</sub>**

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.7087921599  | 0.8068432434  | 0.4595868273  |
| N2  | 1.7496582852  | 0.8539398089  | -0.4397219106 |
| C3  | 0.9448446497  | 1.9195770024  | -0.2428584394 |
| C4  | -0.3276628434 | 1.9928583836  | -0.8158500365 |
| C5  | -0.7717284132 | 0.9501100834  | -1.6236828753 |
| C6  | 0.0520536497  | -0.1591462891 | -1.7991428980 |
| C7  | 1.2965797957  | -0.1890883063 | -1.1673302744 |
| H8  | -0.9500803526 | 2.8621553048  | -0.6285670882 |
| H9  | -1.7507905655 | 0.9920295106  | -2.0928695471 |
| H10 | -0.2698283240 | -1.0095360036 | -2.3921055378 |
| C11 | 1.4688472801  | 3.0200706513  | 0.6360083621  |
| H12 | 0.8945850166  | 3.9382004927  | 0.4865882949  |

|     |              |               |               |
|-----|--------------|---------------|---------------|
| H13 | 1.3469758849 | 2.6921266196  | 1.6774672141  |
| C14 | 2.1691352154 | -1.4180186131 | -1.2102368791 |
| H15 | 1.5802668193 | -2.2871700364 | -1.5183226942 |
| H16 | 2.9669465937 | -1.2778061942 | -1.9497780371 |
| P17 | 3.3119819256 | 3.2417785761  | 0.4751418434  |
| P18 | 3.0663019962 | -1.6435833422 | 0.4187068227  |
| C19 | 1.7099211115 | -2.3651912614 | 1.5763464256  |
| C20 | 4.2967549664 | -3.0416128634 | -0.0388662255 |
| C21 | 3.6352258528 | 4.5104285733  | 1.8869035732  |
| C22 | 3.4989420644 | 4.1468631004  | -1.2145164497 |
| C25 | 2.8608017306 | 3.2501902545  | -2.3027765502 |
| H26 | 3.2076576166 | 2.2177975532  | -2.2389795753 |
| H27 | 1.7698923725 | 3.2445719819  | -2.2418559444 |
| H28 | 3.1285010029 | 3.6453228505  | -3.2914699251 |
| C29 | 2.8361556961 | 5.5328980703  | -1.3060812891 |
| H30 | 1.7703454822 | 5.4952905835  | -1.0574416523 |
| H31 | 3.3136166809 | 6.2688442210  | -0.6556412343 |
| H32 | 2.9151768058 | 5.9085012083  | -2.3353639304 |
| C33 | 5.0032918874 | 4.2755267943  | -1.5444099843 |
| H34 | 5.1203039088 | 4.6011904775  | -2.5866152963 |
| H35 | 5.5121881917 | 5.0082542542  | -0.9178225076 |
| H36 | 5.5174904800 | 3.3195477318  | -1.4262081139 |
| C37 | 2.5030008182 | 5.5400868835  | 2.0902203505  |
| H38 | 2.2869733224 | 6.1347314825  | 1.2012414956  |
| H39 | 1.5753415252 | 5.0609719927  | 2.4157749336  |
| H40 | 2.7971670334 | 6.2358175328  | 2.8865262140  |
| C41 | 3.7912540177 | 3.7218519715  | 3.2063174428  |
| H42 | 2.8881037087 | 3.1725600887  | 3.4766915958  |
| H43 | 4.6070550345 | 2.9975651221  | 3.1569444953  |
| H44 | 4.0066257420 | 4.4347673365  | 4.0131712544  |
| C45 | 4.9628812839 | 5.2520662808  | 1.6344512959  |
| H46 | 5.2320083743 | 5.8166560684  | 2.5356778585  |
| H47 | 5.7826672348 | 4.5560215922  | 1.4272232062  |
| H48 | 4.8968290484 | 5.9697320178  | 0.8128515723  |
| C49 | 5.4836122956 | -2.3507474565 | -0.7437232493 |
| H50 | 5.1856809884 | -1.9034341388 | -1.6967938177 |
| H51 | 5.9152338036 | -1.5640075401 | -0.1203408253 |
| H52 | 6.2609042188 | -3.0957082441 | -0.9586295594 |
| C53 | 3.7550810613 | -4.1322699707 | -0.9853557144 |
| H54 | 3.4308212912 | -3.7182379279 | -1.9453829293 |
| H55 | 4.5559833532 | -4.8520203180 | -1.2003524202 |
| H56 | 2.9213334920 | -4.6912299827 | -0.5605874998 |
| C57 | 4.8417489503 | -3.6936238314 | 1.2475842403  |
| H58 | 5.6928781864 | -4.3386159264 | 0.9940962609  |
| H59 | 5.1925282300 | -2.9426913975 | 1.9630772064  |
| H60 | 4.0967689006 | -4.3206905773 | 1.7425916616  |

|     |               |               |               |
|-----|---------------|---------------|---------------|
| C61 | 1.1918133183  | -3.7555091948 | 1.1639763087  |
| H62 | 0.8330537966  | -3.7793009287 | 0.1289852436  |
| H63 | 1.9454884326  | -4.5371895570 | 1.2863854957  |
| H64 | 0.3422978041  | -4.0248003218 | 1.8052576858  |
| C65 | 0.5067034095  | -1.3915768147 | 1.5872796645  |
| H66 | -0.0365354351 | -1.3905334740 | 0.6387370298  |
| H67 | -0.1965367325 | -1.7277895800 | 2.3601493080  |
| H68 | 0.8132237135  | -0.3753835919 | 1.8403898326  |
| C69 | 2.2521682613  | -2.4251511221 | 3.0238026902  |
| H70 | 1.4583804592  | -2.8149011994 | 3.6749708926  |
| H71 | 3.1133068536  | -3.0851984519 | 3.1344231104  |
| H72 | 2.5181807185  | -1.4318680241 | 3.3885718117  |
| N84 | 4.9122199293  | 0.7634117439  | -1.0829331090 |
| C85 | 5.7308352267  | 0.7800517485  | -1.9097426862 |
| C86 | 6.7875243139  | 0.8078080614  | -2.9116361269 |
| H87 | 6.7762654152  | 1.7628620599  | -3.4467176451 |
| H88 | 7.7635851272  | 0.6874685912  | -2.4297778696 |
| H89 | 6.6537927622  | -0.0031767140 | -3.6348311001 |
| C83 | 3.3331712933  | 0.7890057112  | 2.3315823733  |
| O84 | 4.5655789270  | 0.6000939645  | 2.5167080602  |
| O85 | 2.3361606201  | 0.9155547037  | 3.0515586530  |

$[(P^C N^C P)Co^{II}(NCCH_3)H]^+$

|     |               |               |               |
|-----|---------------|---------------|---------------|
| Co1 | 3.5952874009  | 0.8074461092  | 0.6322989134  |
| N2  | 1.6652890399  | 0.8453205790  | -0.4152867106 |
| C3  | 1.0001351907  | 2.0108959315  | -0.5749414005 |
| C4  | -0.1059033773 | 2.1175127314  | -1.4175345645 |
| C5  | -0.5338992392 | 0.9925866511  | -2.1184632783 |
| C6  | 0.1725286465  | -0.1981811942 | -1.9751756187 |
| C7  | 1.2771243455  | -0.2370184994 | -1.1235267915 |
| H8  | -0.6166703316 | 3.0694491534  | -1.5194911540 |
| H9  | -1.3944556184 | 1.0481105985  | -2.7783117771 |
| H10 | -0.1128742359 | -1.0883198379 | -2.5262035875 |
| C11 | 1.5234860591  | 3.1903963172  | 0.1987100903  |
| H12 | 1.2414263781  | 4.1329095220  | -0.2791665454 |
| H13 | 1.0630408616  | 3.1924644133  | 1.1930561613  |
| C14 | 2.1274683554  | -1.4800838684 | -1.0230740262 |
| H15 | 1.5070063064  | -2.3810607748 | -0.9961367608 |
| H16 | 2.7341541458  | -1.5442951317 | -1.9338343198 |
| P17 | 3.3659981618  | 3.0556692416  | 0.4675633260  |
| P18 | 3.3199620792  | -1.3924056806 | 0.3891557296  |
| C19 | 2.3279600499  | -2.0860829806 | 1.8653062640  |
| C20 | 4.7101153694  | -2.5618821777 | -0.1466009646 |
| C21 | 3.5702350183  | 4.0747544030  | 2.0579218937  |
| C22 | 4.1358303981  | 3.8913887944  | -1.0468841326 |
| C25 | 3.4942310260  | 3.2282088882  | -2.2879011799 |

|     |              |               |               |
|-----|--------------|---------------|---------------|
| H26 | 3.5707605063 | 2.1384395081  | -2.2421920618 |
| H27 | 2.4417574088 | 3.5026958292  | -2.4083640306 |
| H28 | 4.0243203184 | 3.5704674400  | -3.1837561412 |
| C29 | 3.9132156767 | 5.4123348460  | -1.1222205722 |
| H30 | 2.8545582802 | 5.6854453143  | -1.0614591761 |
| H31 | 4.4549917231 | 5.9494927804  | -0.3401333418 |
| H32 | 4.2863180949 | 5.7796075847  | -2.0854282308 |
| C33 | 5.6465118819 | 3.5755638123  | -1.0557103688 |
| H34 | 6.0894009016 | 3.9682657179  | -1.9782484287 |
| H35 | 6.1745459087 | 4.0361692079  | -0.2172204919 |
| H36 | 5.8168152390 | 2.4958904893  | -1.0241615690 |
| C37 | 2.7798538708 | 5.4002616221  | 2.0742479005  |
| H38 | 3.1083466965 | 6.0995381452  | 1.3055553699  |
| H39 | 1.7032015308 | 5.2469451772  | 1.9574101738  |
| H40 | 2.9283733612 | 5.8881809856  | 3.0448510737  |
| C41 | 3.0411205502 | 3.1823190251  | 3.2078361208  |
| H42 | 1.9790649714 | 2.9380544342  | 3.0949046450  |
| H43 | 3.5970555715 | 2.2460155953  | 3.2896315096  |
| H44 | 3.1435344199 | 3.7206988203  | 4.1572836385  |
| C45 | 5.0641283160 | 4.3644072351  | 2.3013240330  |
| H46 | 5.1929870180 | 4.7863723027  | 3.3048515906  |
| H47 | 5.6706369293 | 3.4564190098  | 2.2358736532  |
| H48 | 5.4596480766 | 5.0935681776  | 1.5896636788  |
| C49 | 5.5813540037 | -1.7837485471 | -1.1592804826 |
| H50 | 5.0126533388 | -1.4577777049 | -2.0360060221 |
| H51 | 6.0232644391 | -0.8925721249 | -0.7087888896 |
| H52 | 6.3853415725 | -2.4403381230 | -1.5124086921 |
| C53 | 4.2039096499 | -3.8533540611 | -0.8245019401 |
| H54 | 3.6382765289 | -3.6476714502 | -1.7376912506 |
| H55 | 5.0685469792 | -4.4609969301 | -1.1152726577 |
| H56 | 3.5823694187 | -4.4643368527 | -0.1695475690 |
| C57 | 5.5858539477 | -2.9248404397 | 1.0697105719  |
| H58 | 6.4761297285 | -3.4617350348 | 0.7225879139  |
| H59 | 5.9227171492 | -2.0316784095 | 1.6052902964  |
| H60 | 5.0677641401 | -3.5790993595 | 1.7753531373  |
| C61 | 2.0064956213 | -3.5878370165 | 1.7743568707  |
| H62 | 1.4909029321 | -3.8481987267 | 0.8444367009  |
| H63 | 2.9002476949 | -4.2099448122 | 1.8588641370  |
| H64 | 1.3399059494 | -3.8634149045 | 2.6005806328  |
| C65 | 0.9946827127 | -1.3021212332 | 1.9261546651  |
| H66 | 0.3445286620 | -1.5066104142 | 1.0708502174  |
| H67 | 0.4497729065 | -1.6011307463 | 2.8286291438  |
| H68 | 1.1560665604 | -0.2209603817 | 1.9752881403  |
| C69 | 3.0940850535 | -1.7895209695 | 3.1732180812  |
| H70 | 2.4929039009 | -2.1255629184 | 4.0263734061  |
| H71 | 4.0562634089 | -2.3024647109 | 3.2269152705  |

|     |              |               |              |
|-----|--------------|---------------|--------------|
| H72 | 3.2751707656 | -0.7174455826 | 3.2933618416 |
| N73 | 5.0907856650 | 0.7234061769  | 2.0622134191 |
| C74 | 6.0623884846 | 0.6465552675  | 2.6914381368 |
| C80 | 7.2931011036 | 0.5484512158  | 3.4660700558 |
| H81 | 8.1457132389 | 0.4125512280  | 2.7934215354 |
| H82 | 7.4435318718 | 1.4618174598  | 4.0493340230 |
| H83 | 7.2397984447 | -0.3048792931 | 4.1488458183 |
| H77 | 4.3822755891 | 0.7721124660  | -0.642392804 |

Table S3. Calculations for DFT energies.

| Molecule                    | ZPE<br>[kcal/mol] | Hvib  | Svib   | 6kT | 1/2<br>(Strans+Srot)<br>+ Selec | Selec | Htot | Stot  | D3<br>Correction | E (B3LYP-<br>D3, Acn) | G<br>(Acetonitrile) | # basis     | S*(S+1) | S^2  | S (ideal) | a (mixing) | Projected<br>Energy | NRG Diff<br>(kcal/mol) |
|-----------------------------|-------------------|-------|--------|-----|---------------------------------|-------|------|-------|------------------|-----------------------|---------------------|-------------|---------|------|-----------|------------|---------------------|------------------------|
| PONOP                       |                   |       |        |     |                                 |       |      |       |                  |                       |                     |             |         |      |           |            |                     |                        |
| Co2.(Ace)2                  | 421.53            | 24.71 | 159.80 |     | 3.55                            | 42.05 | 1.38 | 27.08 | 243.17           | -0.12                 | -2122.54            | -1331603.03 | 1123.00 |      |           |            |                     |                        |
| Co2.(Ace)2a doublet SP      | 421.53            | 24.71 | 159.80 |     | 3.55                            | 42.05 | 1.38 | 27.08 | 243.17           | -0.20                 | -2122.46            | -1331606.04 | 1123.00 | 0.75 | 0.77      | 0.50       | 0.01                | -2122.46               |
| Co2.(Ace)2 quartet SP       | 421.53            | 24.71 | 159.80 |     | 3.55                            | 42.05 | 1.38 | 27.08 | 243.17           | -0.20                 | -2122.43            | -1331585.28 | 1123.00 | 3.75 | 3.77      |            |                     | -0.12                  |
| Co2.CoAce                   | 390.89            | 21.87 | 140.64 |     | 3.55                            | 41.73 | 1.38 | 24.24 | 223.84           | -0.11                 | -1989.73            | -1248282.15 | 1036.00 |      |           |            |                     |                        |
| Co2.AceCO2 quartet          | 398.30            | 24.29 | 163.89 |     | 3.55                            | 43.49 | 2.76 | 26.66 | 243.62           | -0.12                 | -2178.35            | -1366644.37 | 1102.00 |      |           |            |                     |                        |
| Co1.(Ace)2 triplet          | 419.22            | 25.59 | 168.47 |     | 3.55                            | 42.92 | 2.18 | 27.96 | 254.64           | -0.12                 | -2122.69            | -1331699.42 | 1123.00 |      |           |            |                     |                        |
| Co1.CoAce trip              | 389.09            | 22.66 | 149.75 |     | 3.55                            | 42.60 | 2.18 | 25.03 | 236.26           | -0.11                 | -1989.88            | -1248377.95 | 1036.00 |      |           |            |                     |                        |
| Co3.CoHAce2 sing            | 427.78            | 24.51 | 157.58 |     | 3.55                            | 40.66 | 0.00 | 26.88 | 239.66           | -0.13                 | -2123.11            | -1331958.02 | 1130.00 |      |           |            |                     |                        |
| Co1.CoAceCO2a trip          | 398.24            | 24.15 | 163.46 |     | 3.55                            | 42.88 | 2.18 | 26.52 | 242.62           | -0.12                 | -2178.51            | -1366750.00 | 1102.00 |      |           |            |                     |                        |
| Co0.Ace1 Carbon bound       | 389.33            | 21.83 | 137.18 |     | 3.55                            | 41.71 | 1.38 | 24.20 | 220.55           | -0.11                 | -1989.96            | -1248429.96 | 1036.00 |      |           |            |                     |                        |
| Co0.Ace2 SP Doublet C bound | 389.33            | 21.83 | 137.18 |     | 3.55                            | 41.71 | 1.38 | 24.20 | 220.55           | -0.11                 | -1990.06            | -1248489.48 | 1036.00 | 0.75 | 0.97      | 0.50       | 0.07                | -1990.06               |
| Co0.Ace2 SP Quartet C bound | 389.33            | 21.83 | 137.18 |     | 3.55                            | 41.71 | 1.38 | 24.20 | 220.55           | -0.11                 | -1990.02            | -1248464.37 | 1036.00 | 3.75 | 3.77      |            |                     | -1.99                  |
| Co0.Co(Ace)2 N bound        | 416.54            | 25.78 | 170.15 |     | 3.55                            | 42.10 | 1.38 | 28.15 | 255.31           | -0.12                 | -2122.75            | -1331743.11 | 1123.00 |      |           |            |                     |                        |
| Co0.(Ace)2b doub SP         | 389.33            | 21.83 | 137.18 |     | 3.55                            | 41.71 | 1.38 | 24.20 | 220.55           | -0.02                 | -2122.85            | -1331764.03 | 1123.00 | 0.75 | 1.53      | 0.50       | 0.26                | -2122.86               |
| Co0.(Ace)2b quartet SP      | 389.33            | 21.83 | 137.18 |     | 3.55                            | 41.71 | 1.38 | 24.20 | 220.55           | -0.02                 | -2122.84            | -1331754.93 | 1123.00 | 3.75 | 3.80      |            |                     | -3.17                  |
| Co0.AceCO2 doublet          | 398.00            | 24.02 | 151.91 |     | 3.55                            | 42.01 | 1.38 | 26.39 | 235.30           | -0.13                 | -2178.63            | -1366826.25 | 1102.00 |      |           |            |                     |                        |
| Co0.CoAceCO2b doublet SP    | 389.33            | 21.83 | 137.18 |     | 3.55                            | 41.71 | 1.38 | 24.20 | 220.55           | -0.03                 | -2178.73            | -1366832.64 | 1102.00 | 0.75 | 1.04      | 0.50       | 0.10                | -2178.73               |
| Co0.CoAceCO2b quartet SP    | 389.33            | 21.83 | 137.18 |     | 3.55                            | 41.71 | 1.38 | 24.20 | 220.55           | -0.03                 | -2178.68            | -1366800.54 | 1102.00 | 3.75 | 3.78      |            |                     | -3.38                  |
| Co2.CoHAce                  | 395.75            | 22.19 | 141.85 |     | 3.55                            | 41.77 | 1.38 | 24.56 | 225.93           | -0.11                 | -1990.46            | -1248737.83 | 1043.00 |      |           |            |                     |                        |
| PNP                         |                   |       |        |     |                                 |       |      |       |                  |                       |                     |             |         |      |           |            |                     |                        |
| Co2.CoAce2                  | 452.41            | 24.81 | 158.66 |     | 3.55                            | 42.06 | 1.38 | 27.18 | 241.65           | -0.13                 | -2050.66            | -1286472.70 | 1151.00 | 0.75 | 0.77      | 0.50       | 0.01                | -2050.66               |
| Co2.CoAce2 SP Doublet       | 452.41            | 24.81 | 158.66 |     | 3.55                            | 42.06 | 1.38 | 27.18 | 241.65           | -0.20                 | -2050.59            | -1286472.70 | 1152.00 | 3.75 | 3.76      |            |                     | -0.28                  |
| Co2.CoAce2 SP quartet       | 452.41            | 24.81 | 158.66 |     | 3.55                            | 42.06 | 1.38 | 27.18 | 241.65           | -0.20                 | -2050.56            | -1286454.05 | 1153.00 |      |           |            |                     |                        |
| Co2.CoAceCO2a               | 430.09            | 23.87 | 156.32 |     | 3.55                            | 42.05 | 1.38 | 26.24 | 233.73           | -0.13                 | -2106.47            | -1321514.17 | 1130.00 |      |           |            |                     |                        |
| Co1.CoAce2                  | 449.84            | 25.58 | 166.66 |     | 3.55                            | 42.90 | 2.18 | 27.95 | 251.15           | -0.13                 | -2050.80            | -1286561.72 | 1151.00 |      |           |            |                     |                        |
| Co1.CoAce1CO2a sing         | 430.49            | 23.78 | 149.06 |     | 3.55                            | 40.61 | 0.00 | 26.15 | 230.64           | -0.14                 | -2106.61            | -1321603.60 | 1130.00 |      |           |            |                     |                        |
| Co3.CoHAce2 sing            | 458.77            | 24.48 | 155.10 |     | 3.55                            | 40.66 | 0.00 | 26.85 | 236.42           | -0.14                 | -2051.24            | -1286831.08 | 1158.00 |      |           |            |                     |                        |
| Co0.CoAce2 N bound          | 446.62            | 25.85 | 168.80 |     | 3.55                            | 42.09 | 1.38 | 28.22 | 252.71           | -0.13                 | -2050.85            | -1286601.19 | 1151.00 |      |           |            |                     |                        |
| Co0.CoAce2b doublet SP      | 446.62            | 25.85 | 168.80 |     | 3.55                            | 42.09 | 1.38 | 28.22 | 252.71           | -0.02                 | -2050.97            | -1286601.19 | 1151.00 | 0.75 | 1.64      | 0.50       | 0.30                | -2050.97               |
| Co0.CoAce2b quartet SP      | 446.62            | 25.85 | 168.80 |     | 3.55                            | 42.09 | 1.38 | 28.22 | 252.71           | -0.02                 | -2050.96            | -1286597.28 | 1151.00 | 3.75 | 3.81      |            |                     | -1.65                  |
| Co0.CoAce carbon bound      | 419.89            | 21.82 | 135.16 |     | 3.55                            | 41.72 | 1.38 | 24.19 | 217.43           | -0.12                 | -1918.06            | -1203288.45 | 1064.00 |      |           |            |                     |                        |
| Co0.Ace SP Doublet C bound  | 419.89            | 21.82 | 135.16 |     | 3.55                            | 41.72 | 1.38 | 24.19 | 217.43           | -0.12                 | -1918.16            | -1203351.68 | 1064.00 | 0.75 | 1.00      | 0.50       | 0.08                | -1918.17               |
| Co0.Ace SP Quartet C bound  | 419.89            | 21.82 | 135.16 |     | 3.55                            | 41.72 | 1.38 | 24.19 | 217.43           | -0.12                 | -1918.12            | -1203326.43 | 1064.00 | 3.75 | 3.86      |            |                     | -2.34                  |
| Co0.CoAceCO2a               | 428.92            | 23.93 | 150.49 |     | 3.55                            | 42.07 | 1.38 | 26.30 | 233.82           | -0.13                 | -2106.73            | -1321678.91 | 1130.00 |      |           |            |                     |                        |
| Co0.CoAceCO2a SP doublet    | 428.92            | 23.93 | 150.49 |     | 3.55                            | 42.07 | 1.38 | 26.30 | 233.82           | -0.04                 | -2106.83            | -1321678.91 | 1130.00 | 0.75 | 1.02      | 0.50       | 0.09                | -2106.83               |
| Co0.CoAceCO2a SP quartet    | 428.92            | 23.93 | 150.49 |     | 3.55                            | 42.07 | 1.38 | 26.30 | 233.82           | -0.04                 | -2106.78            | -1321650.51 | 1130.00 | 3.75 | 3.80      |            |                     | -2.84                  |
| Co2.HAce                    | 425.58            | 22.36 | 140.95 |     | 3.55                            | 41.78 | 1.38 | 24.73 | 223.91           | -0.12                 | -1918.56            | -1203592.68 | 1071.00 |      |           |            |                     |                        |
| Co2.HAce Doublet SP         | 425.58            | 22.36 | 140.95 |     | 3.55                            | 41.78 | 1.38 | 24.73 | 223.91           | -0.06                 | -1918.62            | -1203592.68 | 1071.00 | 0.75 | 0.78      | 0.50       | 0.01                | -1918.62               |
| Co2.HAce quartet SP         | 425.58            | 22.36 | 140.95 |     | 3.55                            | 41.78 | 1.38 | 24.73 | 223.91           | -0.06                 | -1918.59            | -1203574.20 | 1071.00 | 3.75 | 3.77      |            |                     | -0.17                  |

